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16. ABSTRACT

Ambient hydrocarbon data were analyzed to derive hydrocarbon speciation for use with the Carbon Bond Four (CB4) and the Carter, Atkinson, Lurmann (CAL) mechanisms. A total of 66 city-years of detailed surface-layer hydrocarbon data (comprising 773 individual analyses) was available. A total of 56 hydrocarbon samples collected aloft was also added to the data base. These data were speciated into the carbon fractions for hydrocarbon species in the CB4 and CAL mechanisms. Fractions for each mechanism are reported for each city-year, for five clusters of city years with similar internal composition, and for the total. The five clusters were determined using two forms of cluster analysis. Multiple regression was also used to confirm the overall average carbon fractions. Four analyses of automobile exhaust from the UNC autoexhaust smog chamber study were also speciated. Recommendations for the default carbon fractions for OZIPM4 are given. Selected simulations for both mechanisms are used to demonstrate the effects of HC composition on ozone predictions. ⟵

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Abstract

This volume reports on the analysis of ambient hydrocarbon data to derive hydrocarbon speciation for use with the Carbon Bond Four and the Carter, Atkinson, Lurmann mechanisms. New data from on-going EPA projects to monitor ambient air for total nonmethane organic carbon and to speciate the hydrocarbon using gas chromatography provided a data base suitable for analysis using a single set of assumptions and speciation guidance from the model developers. This work first reports on the steps needed to convert this data base into a form suitable for such analyses. A total of 66 city-years of detailed HC data (comprising 773 individual analyses) were available. A total of 56 samples from aloft HC data taken by Washington State University using aircraft were also added to the data base. These data were speciated into the carbon fractions for species in the Carbon Bond Four and Carter, Atkinson, Lurmann mechanisms. Fractions for each mechanism are reported for each city-year, for five clusters of city years with similar internal composition, and for the total. The five clusters were determined using two forms of cluster analysis. Multiple regression was also used to confirm the overall average carbon fractions. Four analyses of automobile exhaust from the UNC autoexhaust smog chamber study were also speciated. Recommendations for the default carbon fractions for OZIPM4 are given. Selected simulations for both mechanisms are used to demonstrate the effects of HC composition on ozone predictions.

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We very much appreciate Dr. William Lonneman making available the detailed gas chromatograph data from the EPA study and for being tolerant while we asked what seemed to be a thousand questions. Likewise, we are indebted to Dr. Hal Westberg for sharing his aloft gas chromatographic data before it was in final form.

We also would like to thank the mechanism developers, Dr. M. Gery, Dr .G. Whitten, Dr. W. Carter, and Dr. F. Lurmann, for assistance in answering the questions about speciation of some compounds.

Finally, we thank Dr. Marcia Dodge for suggesting that we work on this project as part of her cooperative agreement.

Introduction

The U.S. EPA has sponsored the development of two different types of photochemical kinetics mechanisms for use in urban and regional oxidant control applications:

- the Carbon Bond Four mechanism (CB4) is based upon a complete representation of all the carbon in the reacting system by the use of mechanism species that represent carbon-carbon bond types,[1] *e.g.*,
  - ▷ single-bonded carbons including those occurring as side-chains on olefins and aromatic species are represented as a 1-carbon PAR,
  - ▷ ethene as itself, *i.e.*, a 2-carbon ETH,
  - ▷ all other terminal-double-bonded carbons as a 2-carbon OLE with PARs added as needed,
  - ▷ all internal-double-bonded carbons as two 2-carbon ALD with PARs added as needed,
  - ▷ mono-alkylbenzenes as a 7-carbon TOL, but ethyl-benzene as TOL+PAR,
  - ▷ di- and tri-alkylbenzenes as a 9-carbon XYL with PARs added as needed,
  - ▷ formaldehyde as itself (HCHO),
  - ▷ all other carbonyl bonds as a 2-carbon ALD with PARs added as needed, and
  - ▷ non-reactive carbon (*e.g.*, ethane) as a 1-carbon NR;
- the Carter, Atkinson, Lurmann surrogate-species mechanism (CAL) does not represent all the carbon in the system as reactive, but uses the nearly explicit chemistry of several species in each class[2,3] *i.e.*,
  - ▷ C_4 and C_5 alkanes as a 4.5-carbon ALK4,
  - ▷ C_6 and greater alkanes as a 7-carbon ALK7,
  - ▷ ethene as itself (ETH, 2-carbons),
  - ▷ terminal alkenes as propene (PRPE, 3-carbons),
  - ▷ internal alkenes as trans-2-butene (TBUT, 4-carbons),
  - ▷ mono-alkylbenzenes as toluene (TOL, 7-carbons),
  - ▷ di-alkylbenzenes as xylene (XYL, 8-carbons),
  - ▷ tri-alkylbenzenes as tri-methyl-benzene, (TMB, 9-carbons),
  - ▷ formaldehyde as itself (FORM),
  - ▷ acetaldheyde as itself (ALD, 2-carbons),

- ▷ higher aldehydes as propionaldehyde (RCHO, 3-carbons),
- ▷ non-reactives as lumped species (NR, 1-carbon),

to represent all the chemistry of the atmospheric mix. Species are assigned to the closest mechanism species on a molecular basis and any carbon number differences are ignored.

Purpose

The purpose of the work described here was to generate a consistent set of hydrocarbon fractions for both mechanisms using a single data base and set of processing programs and assumptions. This was possible because of recent HC analysis work performed at EPA.

As part of its effort to develop guidance for the use of the OZIPM computer program used to calculate HC and NO_x control requirements, the EPA Office of Air Quality and Planning (OAQPS), in cooperation with the EPA Atmospheric Sciences Research Laboratory (ASRL) at RTP and state and local control agencies, conducted a three-year field program to assess NMOC concentrations by a new technique and to study the detailed hydrocarbon composition by high resolution capillary gas chromatography. These data were made available to us for analysis.[4].

Also as part of OAQPS's effort to develop guidance, Washington State University, under the direction of Dr. Hal Westberg, conducted a study of aloft hydrocarbon upwind of urban areas that might be entrained into the urban mixed layer.[5]

Finally, we included as a source, the detailed HC analyses for automobile exhaust from a controlled and un-controlled vehicle that were part of the UNC smog chamber program on autoexhaust reactivity.[6] This was done to provide modelers with a speciation of the hydrocarbon composition for the automobile exhaust in the chamber that would be consistent with the ambient data hydrocarbon composition. A second reason for including these automobile exhaust data is to provide a comparison with city compositions.

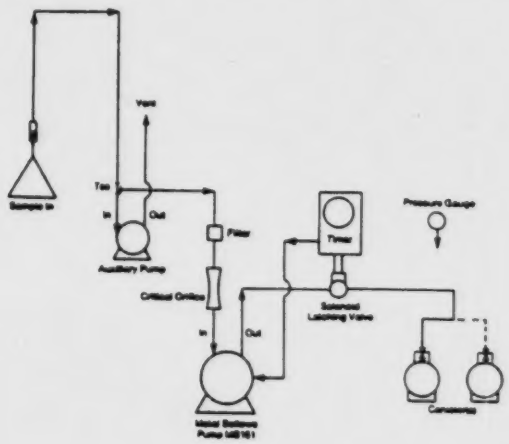

Figure 1. Canister Sampling System (after Dayton *et al.*).

The EPA Data Collection Program

The Methods

The new EPA VOC sampling program was based upon the use of 6-liter SUMMA polished stainless steel spherical canisters to collect integrated ambient air samples which were subsequently shipped to remote laboratories and analyzed by several techniques.[7,8,9] The canisters were cleaned at the laboratory and shipped to the sampling site containing a 5 mm Hg vacuum. At the sampling site, the canisters were filled to 30 or 40 psig over a 3-hour period (0600–0900 LST) by the use of a metal bellows pump and critical orifice (see Figure 1). The storage of NMOC in the canisters has been studied extensively,[10,11] and it was found that there was no significant NMOC concentration change when either the canister pressure was decreased or when the ambient air samples were stored in the canisters for two weeks after the initial analysis. In addition, detailed measurements were made during the clean up procedure, and sample carry over was measured to be less than 0.1% before the final evacuation of the canister.

All canisters were analyzed by the cryogenic preconcentration direct flame ionization detection (PDFID) method at Radian Corporation's Research Triangle Park

Laboratory. In addition, a large number of canisters were subsequently analyzed by the Quality Assurance Division of EPA using the same technique as Radian, and by William Lonneman at EPA's ASRL using a preconcentration system on a fused silica capillary column gas chromatograph. In addition, Lonneman re-analyzed at least one sample from each of the urban areas using chemical stripper columns to remove aromatics and olefins to assist in identification of the peaks. In this way, at least the class of the large number of unidentified compounds could be determined.

The Washington State Field Program for aloft HC used an instrumented aircraft to fly "arcs" upwind of large urban areas. Samples for NMOC were collected over the whole arc (about 10 minutes time) using identical canisters as described above. The canisters were analyzed at the Pullman WA laboratories. Storage times were about four days.

The Sites

The cities and sites were chosen to provide data for use in the EKMA procedure. Thus samples were collected from 6–9 AM on days when the ozone concentration was most likely to be the highest. All monitoring sites were in metropolitan areas, and several were located near petrochemical facilities. Integrated 3-hour samples were taken from early June through September, Monday through Friday, except on holidays, and were analyzed the next day or the following Monday.[12]

Table 1 lists the 47 city-sites (five cities had two sites) included in the 1984, 1985, and 1986 NMOC study and the three or four letter code assigned to each. Not all sites were sampled in all three years of the program, and therefore there were only 66 unique city-site-years in the total data base.

Table 2 lists the cities and dates on which aloft HC sampling was performed.

Table 1. City-Sites For the NMOC Sampling Program and Their Codes.

AKOH	Akron, OH
ATGA	Atlanta, GA
BHAL	Birmingham, AL
BLMD	Baltimore, MD
BMTX	Beaumont, TX
BNY	Brooklyn, NY
BOMA	Boston, MA
BPCT	Bridgeport, CT
BRLA	Baton Rouge, LA
C1IL	Chicago (Site 1), IL
C2IL	Chicago (Site 2), IL
CHNC	Charlotte, NC
CHTN	Chattanooga, TN
CLOH	Cleveland, OH
CLTX	Clute, TX
CNOH	Cincinnati, OH
D1CO	Denver (Site 1), CO
D2CO	Denver (Site 2), CO
DLTX	Dallas, TX
DUNC	Durham, NC
ELTX	El Paso, TX
FWTX	Fort Worth, TX
H1TX	Houston (Site 1), TX
H2TX	Houston (Site 2), TX
ININ	Indianapolis, IN
KCMO	Kansas City, MO
LCLA	Lake Charles, LA
MIFL	Miami, FL
MNY	Manhattan, NY
MTN	Memphis, TN
NHCT	New Haven, CT
ORTX	West Orange, TX
P1PA	Philadelphia (Site 1), PA
P2PA	Philadelphia (Site 2), PA
PHPA	Philadelphia, PA
PTME	Portland, ME
RLNC	Raleigh, NC
RVA	Richmond, VA
S1UT	Salt Lake City (Site 1), UT
S2UT	Salt Lake City (Site 2), UT
SLMO	St. Louis, MO
SWPA	Wilkes-Barre, PA
TCTX	Texas City, TX
TLOK	Tulsa, OK
TRNJ	Trenton, NJ
WDC	Washington, DC
WPFL	West Palm Beach, FL

Table 2. Cities For the NMOC Aloft Sampling Program and Their Codes.

ATLA Atlanta
August 19, 1985 A
August 19, 1985 B2
August 19, 1985 C
August 20, 1985 C1
August 21, 1985 B
August 21, 1985 C1
August 22, 1985 C
August 23, 1985 A

BIRM Birmingham

August 26, 1985 A
August 26, 1985 B
August 28, 1985 A

DALL Dallas

July 8, 1985 B
July 11, 1985 A
July 12, 1985 A
July 12, 1985 C
July 13, 1985 A
July 13, 1985 C

NEWY New York

July 21, 1986 C
July 23, 1986 C
August 5, 1986 B
August 9, 1986 C
August 11, 1986 A
August 11, 1986 B
August 11, 1986 C
August 14, 1986 A

PHIL Philadelphia
July 11, 1986 B
July 25, 1986 C
July 27, 1986 B
July 27, 1986 C
July 30, 1986 C

TULS Tulsa

July 16, 1985 A
July 16, 1985 B
July 16, 1985 C
July 17, 1985 A
July 18, 1985 A
July 18, 1985 B
July 19, 1985 B
July 19, 1985 C
July 20, 1985 A
July 20, 1985 B
July 20, 1985 C
July 21, 1985 B
July 21, 1985 C
July 22, 1985 A
July 22, 1985 B1
July 22, 1985 B2
July 23, 1985 A
July 23, 1985 B
July 23, 1985 C1
July 23, 1985 C3
July 24, 1985 B
July 24, 1985 C1

The EPA NMOC Results

Some of the results from the 1985 portion of the NMOC study[12] will be presented here to provide a context for our subsequent analyses.

Nineteen sites were included in the 1985 study. The precision of the NMOC data was excellent: on repeated analysis of 155 samples, the average difference was 0.49%, and the average absolute difference was 10.5% with a standard deviation of 13.4%. In addition, 131 full duplicate samples were analyzed (*i.e.*, two canisters were collected); the precision for these duplicate was 1.69%, with an average absolute difference of 12.4% and a standard deviation of 17.3%. The agreement among all three laboratories was also excellent: the EPA-QAD concentrations averaged 8.9% higher than the Radian results, and the EPA-ASRL gas chromatographic sum of species concentrations averaged 2.5% lower than the Radian results. A stem-and-leaf plot and summary statistics are shown in Figure 2 taken from McAllister *et al.*[12]. A stem-and-leaf plot is a frequency histogram rotated 90 degrees. The observations are separated into 0.05 ppmC intervals (up to 1.8 ppmC). The numbers to the left of the vertical space (stem) are the concentrations to the nearest 0.1 ppmC and the digits to the right (leaves) are the hundredth of a ppmC for each observation. This plot should be compared with one we will present later for the samples included in our analyses.

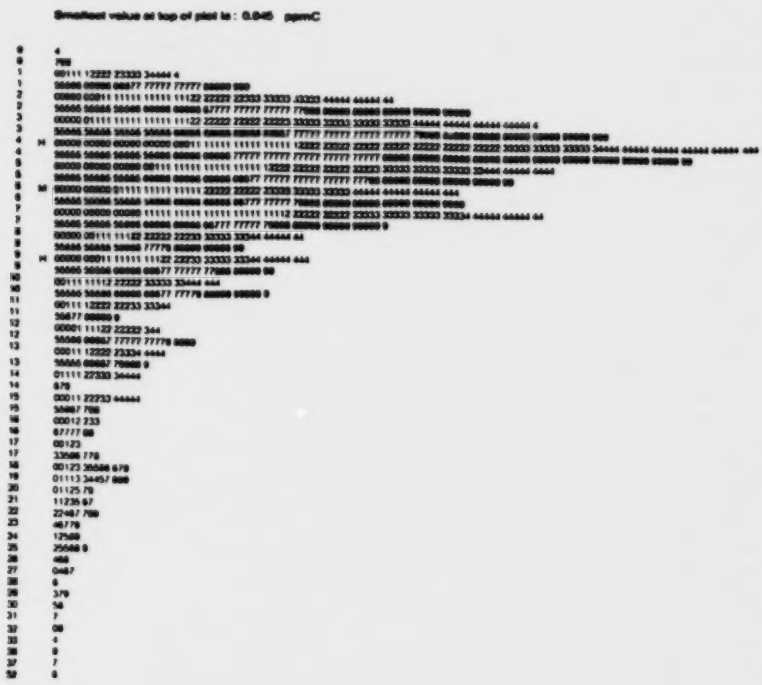

Figure 2. A Stem-and-Leaf Plot of the 1985 NMOC Data, (after McAllister, *et al.*).

	NMOC,ppmC
N OF CASES	1500
MINIMUM	0.045
MAXIMUM	5.267
MEAN	0.755
MEDIAN	0.603
STANDARD DEV	0.541
SKEWNESS	2.186
KURTOSIS	7.232

Data Preparation

EPA-ASRL GC Data

The data we obtained from Lonneman at EPA-ASRL consisted of dBASE files, one for each city-year, that included 860 canister analyses for 1984, 1985, and 1986. We used dBASE to write these canister data to ASCII text files which could be read by other software. In addition, we were supplied a dBASE file that listed the retention times, an EPA-assigned HC identification number and a corresponding species name. This file was converted to a IDTABLE.TXT file. A listing of this table appears in Appendix A. Because the data bases were still in preliminary draft form, we did a quality analysis of the data. This required that we write a number of programs designed to process the data files in various ways, for example, to check that all species identification numbers in the data file had corresponding identification numbers and names in the IDTABLE.TXT file and to find any duplicate numbers. These programs are described in Appendix A. After several passes and consultations with Lonneman, we had "clean" data files.

We wanted a typical composition of the urban mix, and so we used a *trim means* approach.[13] We thus dropped samples with the highest 2% and lowest 2% of total NMOC concentration so that the composition would not be so effected by the extremes. We sorted the species in each remaining canister into decreasing concentration and produced a master list of all the species with concentrations greater than the 21^{st} species in each canister. On the average, in each canister, these 20 species accounted for 66% of the canister's carbon. For each species that occurred in the top 20 compounds in any canister the list included:

- the maximum and minimum fraction observed in the top 20 of any canister,
- the canister identification-numbers associated with these values,
- the average concentration and fraction of each species in all canisters,
- the average concentration and fraction of each species in the canisters in which it appeared,
- and the total number of canisters in which each species appeared.

The initial list had more than 200 compounds that were in the top 20 of the 860 canisters. Many of these compounds, however, only appeared in a few canisters. For example, in the order of the number of canisters for which the species was observed to be in the top 20, the 50^{th} species (1,2-dimethyl-ethyl benzene) appeared in only 18 canisters (2%), the 25^{th} species (3-methyl hexane) appeared in 127 canisters (15%), the 15^{th} species (1,2,4 trimethyl benzene) appeared in 647 canisters (75%), and toluene appeared in the top 20 compounds in all canisters. Examination of the

less common compounds with large concentrations readily showed what appeared to be contamination or highly un-representative samples. One compound, delta-3-carene, appeared randomly in large concentrations in the 1984 samples, with less frequency in the 1985 samples, and hardly at all in the 1986 samples. We assumed that large concentrations of this compound were due to contamination somewhere in the sampling and handling process and that canisters with delta-3-carene in the top 20 should be eliminated from the analyses. In addition, some samples were obviously taken very near venting of process streams in some of the petrochemical facilities, and all canisters in which a single compound represent more than 50% of the total carbon were eliminated. In a seven-cycle process of elimination of these suspect canisters and reforming the top 20 master list, the data base was reduced to 773 canisters for 66 city-years. The master list of the top 20 compounds for the 773 canisters is given in Table 3.

WSU Aloft GC Data

These data were in the form of tables in the final report[5]. We entered the tabular data into a spreadsheet program and produced ASCII files with formats identical to those above. These data also required a quality check and were subjected to a treatment similar to that described above for Lonneman's data. The criteria to select samples were:

1. the sample had to contain greater than 15 ppbC;
2. the sample had to have more thab 80% of the NMOC speciated;
3. the sample had to include aldehyde data; and
4. the sample could not contain large fractions ($> 30\%$) for any single species.

The application of these criteria resulted in the selection of 53 canisters out of the total of 160 canisters collected. It should be noted that the tabular data reported by Westberg and MacGregor require a calibration adjustment by multiplying all values by 1.14 (except for the aldehydes). In the data sets supplied with our report this correction has already been done.

Table 3. Master List of the Top-20 Compounds for 773 Canisters.

ALLCITY.LIS Number of Canisters = 773 #84: 195 #85: 275 #86: 303

Ave NMHC (ppbC) = 761.0 Max NMHC = 2764.6 Min NMHC = 175.7
Ave Frac of Total = 66.3% Max Frac = 90.5% Min Frac = 48.8%

	ID#	Name	TMean	ppbC	EMean	ppbC	Max	Min	#Obs	#84	#85	#86	MaxCan	City	Yr	MinCan	City	Yr
1	185	TOLUENE	6.0%	45.4	5.96%	45.4	18.7%	1.1%	773	100.0%	100.0%	100.0%	2837	C11L	86	2600	CLTX	85
2	124	n-PENTANE	3.7%	27.9	3.65%	27.8	16.0%	0.8%	769	100.0%	98.9%	99.7%	2303	FWTX	86	1212	CLTX	85
3	119	ISOPENTANE	7.4%	56.5	7.38%	56.1	19.4%	0.7%	768	99.5%	98.5%	100.0%	2608	TCTX	85	1212	CLTX	85
4	115	n-BUTANE	7.1%	54.3	7.07%	53.8	22.4%	1.8%	766	100.0%	97.5%	100.0%	1872	BMTX	84	1074	CLTX	85
5	215	m&p-XYLENE	3.3%	24.6	3.17%	24.2	12.4%	0.6%	758	97.9%	96.0%	100.0%	1608	WDC	85	1787	CLTX	85
6	141	2-METHYLPENTANE	2.5%	19.1	2.44%	18.6	5.6%	0.8%	753	96.9%	96.4%	98.7%	1862	H1TX	85	2600	CLTX	85
7	101	ETHANE	4.4%	33.3	4.25%	32.4	22.5%	1.1%	752	95.4%	99.3%	96.7%	1930	TCTX	84	1375	PTHE	85
8	102	ETHYLENE	3.9%	29.1	3.69%	28.1	30.3%	0.9%	746	99.0%	91.6%	99.3%	2099	BMTX	86	1671	BMTX	84
9	162	BENZENE	2.2%	17.0	2.15%	16.4	9.4%	0.7%	745	94.4%	94.5%	99.3%	2452	NNCT	86	1930	TCTX	84
10	105	PROPANE	5.0%	37.6	4.72%	35.9	25.6%	1.1%	739	95.9%	93.5%	97.4%	1483	ORTX	85	2182	RLNC	85
11	145	3-METHYLPENTANE	1.8%	14.0	1.70%	12.9	6.2%	0.7%	712	94.4%	90.5%	92.1%	2450	CHTN	84	1248	H1TX	85
12	110	ISOBUTANE	3.3%	24.8	2.99%	22.7	21.7%	1.1%	707	82.6%	92.4%	96.4%	1185	BMTX	85	2181	KCMO	84
13	148	n-HEXANE,2-ETHYL-1-BUTENE	2.0%	15.8	1.82%	13.9	8.5%	1.1%	678	91.3%	93.5%	80.2%	1640	ORTX	84	1185	BMTX	85
14	103	ACETYLENE	2.6%	19.3	2.18%	16.6	12.3%	0.7%	665	90.3%	80.0%	88.8%	2689	DLTX	86	2471	BMTX	84
15	253	1,2,4-TRIMETHYLBENZENE	2.0%	14.8	1.62%	12.4	7.4%	0.8%	647	76.9%	73.1%	97.7%	2234	TLOK	86	2612	BMTX	85
16	222	o-XYLENE	1.5%	11.0	0.91%	6.9	4.2%	0.7%	485	30.3%	59.3%	86.8%	2234	TLOK	86	2151	BRLA	85
17	173	2,2,4-TRIMETHYLPENTANE	1.5%	12.1	0.86%	6.6	2.4%	0.6%	420	47.7%	50.5%	62.0%	2099	BRLA	85	1212	CLTX	85
18	104	PROPENE	2.1%	17.2	1.21%	9.2	20.2%	0.8%	414	41.5%	54.9%	60.1%	1248	H1TX	85	2219	CLDH	85
19	166	2-METHYLHEXANE	1.5%	11.3	0.73%	5.5	3.4%	0.7%	379	27.7%	62.5%	50.5%	2542	KCMO	85	1930	TCTX	84
20	252	p,m,o-METHYLSTYRENE	2.6%	16.3	0.85%	6.4	15.8%	0.6%	306	87.7%	47.3%	1.7%	1820	RVA	84	1787	CLTX	85
21	113	2-METHYLPROPENE,BUTENE-1	1.5%	11.2	0.42%	3.2	9.3%	0.7%	221	14.9%	23.6%	41.9%	2415	KCMO	85	2471	BMTX	84
22	156	METHYLCYCLOPENTANE	1.4%	12.8	0.44%	3.3	14.2%	0.7%	202	32.3%	31.3%	17.5%	1717	LCLA	85	1417	LCLA	85
23	213	ETHYLBENZENE	1.6%	13.7	0.34%	2.6	18.1%	0.9%	146	10.3%	17.8%	25.4%	2648	H1TX	85	1156	KCMO	85
24	356	C10 AROMATIC	2.0%	9.7	0.21%	1.6	5.4%	0.8%	128	0.0%	6.5%	36.3%	2468	BPCT	86	1998	TLOK	86
25	170	3-METHYLHEXANE	1.4%	11.8	0.26%	1.9	4.2%	0.8%	127	41.5%	8.4%	7.6%	1360	WPFL	84	1930	TCTX	84
26	0	unknown	2.2%	14.4	0.30%	2.3	15.0%	0.6%	123	27.7%	15.3%	8.9%	2557	DLTX	86	1417	LCLA	85
27	355	C11 OLEFIN	2.0%	10.7	0.21%	1.6	7.6%	0.6%	113	38.5%	12.4%	1.3%	1361	ELTX	84	1787	CLTX	85
28	175	n-HEPTANE	1.3%	13.1	0.23%	1.7	3.3%	0.6%	102	10.3%	10.5%	17.5%	1367	DLTX	85	1316	LCLA	85
29	244	m-ETHYLTOLUENE	1.4%	10.3	0.17%	1.3	2.5%	1.1%	99	6.2%	10.5%	19.1%	1490	CHTN	84	2241	BHAL	84
30	167	2,3-DIMETHYLPENTANE	1.7%	14.3	0.19%	1.4	3.6%	0.9%	76	0.5%	5.8%	19.5%	1365	C2IL	86	1894	TLOK	86
31	260	1,2,3-TRIMETHYLBENZENE	4.1%	30.2	0.38%	2.9	21.8%	0.6%	73	9.2%	19.6%	0.3%	1156	KCMO	85	1417	LCLA	85
32	256	n-DECANE	1.7%	13.6	0.16%	1.3	3.5%	0.8%	71	2.6%	8.7%	13.9%	1829	C2IL	86	2471	BMTX	84
33	239	a-PINENE	4.9%	45.3	0.45%	3.5	16.3%	0.9%	59	4.6%	15.3%	2.6%	2160	BMTX	85	2300	LCLA	85
34	179	METHYLCYCLOHEXANE	1.3%	12.2	0.11%	0.8	7.2%	0.7%	52	9.7%	7.6%	4.0%	1367	DLTX	85	1417	LCLA	85
35	164	CYCLOHEXANE	3.2%	28.1	0.21%	1.6	20.6%	0.6%	43	7.7%	6.5%	3.3%	1570	BMTX	86	1316	LCLA	85
36	192	C8 PARAFFIN	1.7%	12.9	0.09%	0.7	4.5%	0.7%	42	14.4%	4.7%	0.3%	1360	WPFL	84	1257	TCTX	84
37	261	1-METHYL-4-ISOPROPYLBENZENE	2.3%	13.6	0.10%	0.7	7.1%	0.9%	42	0.0%	11.3%	3.6%	1274	RVA	85	1638	H1TX	85
38	132	C6 PARAFFIN	2.9%	14.4	0.10%	0.8	9.3%	1.2%	41	5.6%	8.4%	2.3%	2066	DLTX	85	1239	FWTX	84
39	220	C9 OLEFIN	6.2%	53.4	0.35%	2.7	13.6%	0.7%	39	1.5%	9.1%	3.6%	1059	BMTX	85	1212	CLTX	85
40	264	C10 AROMATIC	2.4%	25.0	0.16%	1.2	4.8%	1.0%	37	4.1%	6.9%	3.3%	2294	BMTX	85	2492	TCTX	85
41	301	C11 AROMATIC	1.8%	8.8	0.05%	0.4	5.6%	0.9%	33	11.8%	3.3%	0.3%	1644	SWPA	84	1774	ORTX	84
42	279	C11 PARAFFIN	2.7%	10.4	0.05%	0.4	11.5%	0.7%	29	0.0%	1.1%	8.6%	2397	PHPA	86	2600	CLTX	85
43	158	2,2,3-TRIMETHYL-1-BUTENE	2.0%	14.7	0.06%	0.5	8.3%	0.6%	26	5.6%	2.2%	3.0%	1523	BHAL	84	1212	CLTX	85
44	300	C11 AROMATIC	1.9%	22.1	0.09%	0.7	6.5%	0.8%	25	2.6%	4.4%	2.6%	1894	SLMO	85	1483	ORTX	85
45	251	C10 PARAFFIN	2.8%	29.6	0.13%	1.0	5.1%	0.9%	25	0.5%	7.6%	1.0%	2160	BMTX	85	1570	BMTX	86
46	125	ISOPRENE	1.9%	8.8	0.04%	0.3	6.0%	1.0%	25	5.1%	4.0%	1.3%	2369	RLNC	85	2300	LCLA	85
47	129	c-2-PENTENE	2.0%	17.3	0.06%	0.4	10.3%	0.9%	19	1.5%	2.9%	2.6%	2721	H2TX	86	2081	PTHE	85
48	114	1,3-BUTADIENE	3.4%	22.7	0.07%	0.5	10.4%	0.6%	18	3.1%	4.4%	0.0%	1575	ORTX	85	1787	CLTX	85

Table 3. (cont.)

	ID#	Name	TMean	ppbC	EMean	ppbC	Max	Min	#Obs	#84	#85	#86	MaxCan	City	Yr	MinCan	City	Yr
49	199	C9 PARAFFIN	2.2%	17.8	0.05%	0.4	12.6%	1.2%	18	0.0%	2.5%	3.6%	1107	RLNC	85	2481	BHY	86
50	282	1,2-DIMETHYL-3-ETHYLBENZENE	1.8%	12.2	0.04%	0.3	3.8%	1.0%	18	0.5%	1.1%	4.6%	1968	DLTX	86	2125	WDC	86
51	228	n-NONANE	2.2%	17.9	0.05%	0.4	5.4%	1.0%	17	1.5%	3.3%	1.7%	1406	BOMA	85	1515	BRLA	85
52	248	C10 PARAFFIN	2.2%	25.1	0.07%	0.6	10.1%	1.0%	17	5.6%	0.7%	1.3%	2279	ORTX	84	1515	BRLA	85
53	116	t-2-BUTENE	1.5%	15.3	0.04%	0.3	3.5%	0.9%	15	1.0%	3.3%	1.3%	2159	ORTX	85	1872	BMTX	84
54	267	C10 AROMATIC	1.7%	19.8	0.05%	0.4	3.3%	1.0%	15	5.6%	0.0%	1.3%	1490	CHTN	84	2392	CLTX	84
55	221	C9 PARAFFIN	2.0%	10.3	0.02%	0.2	3.1%	1.2%	14	6.2%	0.7%	0.0%	1360	WPFL	84	2294	BMTX	85
56	198	n-OCTANE	3.4%	18.8	0.04%	0.3	10.4%	1.2%	13	0.5%	0.7%	3.3%	1714	WNCT	86	2630	BRLA	85
57	407	C6 PARAFFIN	2.0%	13.2	0.03%	0.2	3.9%	1.2%	12	3.6%	1.5%	0.3%	1716	ORTX	85	1206	RVA	84
58	238	C10 PARAFFIN	1.8%	16.9	0.03%	0.3	4.2%	1.1%	12	0.0%	1.5%	2.6%	1909	BMTX	86	1185	BMTX	85
59	107	PARAFFIN	2.1%	9.3	0.02%	0.1	6.3%	0.9%	12	0.0%	1.8%	2.3%	1825	PHPA	86	2600	CLTX	85
60	998	ILLEGAL NAME	9.8%	121.9	0.23%	1.7	11.7%	5.5%	11	0.0%	4.0%	0.0%	1352	RLNC	85	1102	RLNC	85
61	139	2,3-DIMETHYLBUTANE	1.4%	21.4	0.04%	0.3	2.5%	0.8%	10	3.6%	0.4%	0.7%	1610	BHAL	84	2299	BMTX	86
62	128	2-METHYL-2-BUTENE	2.3%	22.3	0.03%	0.3	11.8%	1.0%	9	0.5%	0.7%	2.0%	2240	PHPA	86	2038	CLTX	84
63	382	C3 PARAFFIN	3.5%	21.6	0.03%	0.3	10.1%	1.2%	9	2.1%	0.7%	1.0%	2151	BRLA	85	2777	TLOK	86
64	347	C7 PARAFFIN	2.4%	11.6	0.02%	0.1	4.0%	1.2%	8	2.6%	0.4%	0.7%	1141	BRLA	85	1314	S1UT	86
65	120	C5 OLEFIN	3.1%	31.9	0.04%	0.3	8.9%	1.3%	8	1.5%	0.7%	1.0%	2296	PTNE	85	1937	BLND	86
66	123	2-METHYL-1-BUTENE	1.2%	9.3	0.01%	0.1	2.0%	0.8%	7	0.0%	1.5%	1.0%	1630	BHAL	86	2831	H1TX	86
67	126	t-2-PENTENE	2.4%	20.7	0.02%	0.2	10.6%	1.0%	7	0.0%	1.1%	1.3%	2449	DLTX	86	1702	H1TX	85
68	231	C10 PARAFFIN	1.7%	9.2	0.01%	0.1	2.1%	1.1%	7	0.0%	2.5%	0.0%	1558	CLOH	85	1542	DLTX	85
69	172	C7 PARAFFIN	1.7%	20.8	0.02%	0.2	4.3%	1.1%	6	2.1%	0.0%	0.7%	1494	ATGA	84	2908	TRNJ	86
70	344	C6 OLEFIN	1.7%	12.8	0.01%	0.1	2.8%	1.0%	6	0.0%	1.5%	0.7%	1248	H1TX	85	2320	BMTX	86
71	229	C10 PARAFFIN	4.9%	31.7	0.03%	0.2	7.7%	2.5%	6	1.0%	1.5%	0.0%	1344	TCTX	84	1617	CHNC	84
72	177	C8 OLEFIN	1.5%	7.7	0.01%	0.1	1.9%	1.3%	6	0.0%	1.5%	0.7%	2940	TLOK	86	1515	BRLA	85
73	144	C6 OLEFIN	2.7%	26.6	0.03%	0.2	8.7%	1.0%	6	1.0%	1.1%	0.3%	1702	H1TX	85	1483	TCTX	84
74	232	ISOPROPYLBENZENE	3.1%	12.8	0.01%	0.1	6.6%	1.2%	6	0.5%	1.5%	0.3%	1430	P2PA	85	2392	CLTX	84
75	163	3,3-DIMETHYLPENTANE	2.3%	10.7	0.01%	0.1	3.4%	0.7%	5	0.0%	1.1%	0.7%	1932	RVA	85	2600	CLTX	85
76	230	C10 PARAFFIN	2.7%	12.0	0.01%	0.1	6.2%	2.0%	5	0.0%	1.8%	0.0%	1464	H1TX	85	1274	RVA	85
77	117	c-2-BUTENE	1.3%	17.4	0.01%	0.1	1.8%	1.0%	5	0.5%	0.7%	0.7%	2428	ELTX	84	2378	S1UT	86
78	369	C6 PARAFFIN	1.8%	11.7	0.01%	0.1	3.4%	1.4%	5	2.1%	0.0%	0.3%	2340	ORTX	84	2368	PHPA	84
79	165	C7 OLEFIN	1.7%	5.4	0.00%	0.0	2.1%	1.3%	5	2.6%	0.0%	0.0%	1564	WPFL	84	1360	WPFL	84
80	143	C6 OLEFIN	1.9%	16.0	0.01%	0.1	2.4%	1.1%	4	2.1%	0.0%	0.0%	1310	ATGA	84	1244	SWPA	84
81	255	C10 PARAFFIN	5.2%	31.9	0.02%	0.2	8.7%	2.1%	4	0.5%	1.1%	0.0%	1212	CLTX	85	1358	CLTX	85
82	383	C3 PARAFFIN	1.8%	21.4	0.01%	0.1	2.4%	0.9%	4	2.1%	0.0%	0.0%	1483	TCTX	84	1616	BMTX	84
83	138	CYCLOPENTANE	1.1%	15.1	0.01%	0.1	1.7%	0.8%	4	1.0%	0.7%	0.0%	2600	CLTX	85	1671	BMTX	84
84	408	delta-3-CARENE	4.4%	51.0	0.03%	0.3	7.4%	1.4%	4	0.5%	1.1%	0.0%	1029	P1PA	85	2006	DLTX	84
85	388	C8 PARAFFIN	1.2%	13.0	0.01%	0.1	1.3%	1.0%	4	0.0%	1.5%	0.0%	1130	BMTX	85	2079	BMTX	85
86	171	C7 PARAFFIN	1.5%	5.5	0.00%	0.0	2.4%	1.1%	4	0.5%	0.0%	1.0%	2397	PHPA	86	1617	CHNC	84
87	263	C11 PARAFFIN	1.1%	3.6	0.00%	0.0	1.3%	0.8%	4	0.0%	1.5%	0.0%	1849	DLTX	85	2600	CLTX	85
88	151	2-METHYL-2-PENTENE	2.4%	20.0	0.01%	0.1	3.0%	1.6%	3	0.5%	0.4%	0.3%	1702	H1TX	85	1723	AKOH	84
89	393	C5 OLEFIN	2.2%	8.2	0.00%	0.0	3.1%	1.4%	3	1.5%	0.0%	0.0%	2489	AKOH	84	1248	RVA	84
90	340	C12 AROMATIC	1.7%	5.8	0.00%	0.0	2.0%	1.2%	3	1.5%	0.0%	0.0%	2323	M1FL	84	2468	ATGA	84
91	236	C10 PARAFFIN	3.7%	32.9	0.02%	0.1	4.7%	1.4%	3	1.0%	0.4%	0.0%	1344	TCTX	84	1360	WPFL	84
92	207	C9 PARAFFIN	1.6%	11.6	0.01%	0.0	2.2%	1.5%	3	0.0%	1.1%	0.0%	1430	P2PA	85	2297	SLNO	85
93	304	C12 PARAFFIN	1.4%	9.0	0.00%	0.0	1.9%	1.1%	3	0.0%	0.7%	0.3%	1932	RVA	85	1243	SLNO	85
94	246	C9 AROMATIC	1.5%	12.5	0.01%	0.0	1.7%	1.2%	3	0.0%	0.0%	1.0%	2789	TRNJ	86	2869	TRNJ	86
95	153	c or t-2-HEXENE	3.8%	22.2	0.01%	0.1	4.2%	3.2%	2	1.0%	0.0%	0.0%	2298	AKOH	84	2159	AKOH	84
96	363	C12 AROMATIC	1.3%	6.3	0.00%	0.0	1.5%	1.2%	2	0.5%	0.4%	0.0%	1237	BRLA	85	1523	BHAL	84
97	193	2,2,5-TRIMETHYLHEXANE	1.1%	6.8	0.00%	0.0	1.5%	1.0%	2	0.0%	0.4%	0.3%	2536	BHAL	86	1074	CLTX	85
98	204	2,4-DIMETHYLHEPTANE	1.6%	3.6	0.00%	0.0	1.7%	1.4%	2	0.0%	0.0%	0.7%	2188	BLND	86	1417	BPCT	86
99	412	C5 OLEFIN	3.3%	59.9	0.02%	0.2	3.4%	3.1%	2	0.5%	0.4%	0.0%	1059	BMTX	85	1471	KCNO	84
100	343	C4 OLEFIN	1.4%	15.7	0.01%	0.0	1.5%	1.4%	2	0.0%	0.7%	0.0%	2399	BMTX	85	2160	BMTX	85
101	142	t-4-METHYL-2-PENTENE	1.3%	8.9	0.00%	0.0	1.3%	1.2%	2	0.0%	0.4%	0.3%	2299	BMTX	86	2502	DLTX	85
102	140	c-4-METHYL-2-PENTENE	2.9%	17.3	0.01%	0.0	3.3%	2.4%	2	0.0%	0.4%	0.3%	1921	H1TX	85	1230	C1IL	86
103	181	2,4-DIMETHYLHEXANE	2.5%	27.9	0.01%	0.1	4.6%	1.5%	2	0.5%	0.4%	0.0%	1617	CHNC	84	1029	P1PA	85
104	269	C10 AROMATIC	1.6%	17.8	0.01%	0.0	2.2%	1.3%	2	0.5%	0.4%	0.0%	1617	CHNC	84	1029	P1PA	85
105	227	C9 PARAFFIN	3.0%	16.5	0.01%	0.0	5.4%	2.0%	2	0.5%	0.4%	0.0%	1102	RLNC	85	2410	CHNC	84
106	273	C11 PARAFFIN	1.6%	20.8	0.01%	0.1	1.7%	1.6%	2	0.5%	0.0%	0.3%	1490	CHTN	84	1600	H2TX	86
107	250	C9 AROMATIC	2.3%	10.3	0.00%	0.0	2.8%	1.6%	2	0.5%	0.0%	0.3%	2445	CLTX	84	2558	H1TX	86
108	367	C9 PARAFFIN	1.7%	16.1	0.01%	0.0	2.0%	1.3%	2	0.0%	0.7%	0.0%	1212	CLTX	85	1787	CLTX	85

Table 3. (cont.)

	ID#	Name	TMean	ppbC	EMean	ppbC	Max	Min	#Obs	#84	#85	#86	MaxCan	City	Yr	MinCan	City	Yr
109	323	C12 AROMATIC	1.5%	8.3	0.00%	0.0	1.7%	1.3%	2	1.0%	0.0%	0.0%	2174	CNOH	84	1700	RVA	84
110	262	C11 PARAFFIN	1.9%	11.6	0.00%	0.0	2.0%	1.7%	2	0.0%	0.7%	0.0%	1579	LCLA	85	1909	ELTX	85
111	226	C9 PARAFFIN	1.9%	11.6	0.00%	0.0	2.2%	1.6%	2	1.0%	0.0%	0.0%	1200	FWTX	84	1334	FWTX	84
112	191	3-METHYLHEPTANE	1.1%	11.0	0.00%	0.0	1.1%	1.1%	2	0.0%	0.7%	0.0%	1457	RLNC	85	1457	RLNC	85
113	404	C12 AROMATIC	3.5%	12.7	0.00%	0.0	3.5%	3.5%	1	0.5%	0.0%	0.0%	1624	ATGA	84	1624	ATGA	84
114	339	C12 AROMATIC	4.1%	10.4	0.00%	0.0	4.1%	4.1%	1	0.5%	0.0%	0.0%	2468	ATGA	84	2468	ATGA	84
115	131	C6 PARAFFIN	5.9%	31.1	0.01%	0.0	5.9%	5.9%	1	0.5%	0.0%	0.0%	1610	BHAL	84	1610	BHAL	84
116	147	C6 OLEFIN	1.5%	7.7	0.00%	0.0	1.5%	1.5%	1	0.5%	0.0%	0.0%	1610	BHAL	84	1610	BHAL	84
117	118	3-METHYL-1-BUTENE	3.9%	44.7	0.01%	0.1	3.9%	3.9%	1	0.0%	0.4%	0.0%	2629	BMTX	85	2629	BMTX	85
118	378	C12 AROMATIC	1.3%	5.1	0.00%	0.0	1.3%	1.3%	1	0.0%	0.4%	0.0%	1237	BRLA	85	1237	BRLA	85
119	184	2,3,4-TRIMETHYLPENTANE	1.2%	2.9	0.00%	0.0	1.2%	1.2%	1	0.0%	0.4%	0.0%	2099	BRLA	85	2099	BRLA	85
120	187	C8 PARAFFIN	1.4%	31.9	0.01%	0.0	1.4%	1.4%	1	0.0%	0.0%	0.3%	2015	C1IL	86	2015	C1IL	86
121	189	2-METHYLHEPTANE	1.0%	24.2	0.00%	0.0	1.0%	1.0%	1	0.0%	0.0%	0.3%	2015	C1IL	86	2015	C1IL	86
122	309	C11 AROMATIC	1.7%	6.6	0.00%	0.0	1.7%	1.7%	1	0.5%	0.0%	0.0%	1323	CHNC	84	1323	CHNC	84
123	203	C9 OLEFIN	2.4%	17.1	0.00%	0.0	2.4%	2.4%	1	0.5%	0.0%	0.0%	1617	CHNC	84	1617	CHNC	84
124	271	C11 PARAFFIN	1.2%	8.6	0.00%	0.0	1.2%	1.2%	1	0.5%	0.0%	0.0%	1617	CHNC	84	1617	CHNC	84
125	265	C10 AROMATIC	1.9%	43.3	0.01%	0.1	1.9%	1.9%	1	0.5%	0.0%	0.0%	2393	CNTN	84	2393	CNTN	84
126	112	Unknown	1.7%	5.3	0.00%	0.0	1.7%	1.7%	1	0.5%	0.0%	0.0%	2149	CLTX	84	2149	CLTX	84
127	216	4-METHYLOCTANE	1.6%	5.4	0.00%	0.0	1.6%	1.6%	1	0.5%	0.0%	0.0%	2392	CLTX	84	2392	CLTX	84
128	338	C12 AROMATIC	1.7%	9.3	0.00%	0.0	1.7%	1.7%	1	0.5%	0.0%	0.0%	2445	CLTX	84	2445	CLTX	84
129	194	1-OCTENE	0.8%	8.1	0.00%	0.0	0.8%	0.8%	1	0.0%	0.4%	0.0%	1074	CLTX	85	1074	CLTX	85
130	380	M-AMYLBENZENE	6.0%	60.9	0.01%	0.1	6.0%	6.0%	1	0.0%	0.4%	0.0%	1212	CLTX	85	1212	CLTX	85
131	366	C8 PARAFFIN	0.6%	5.8	0.00%	0.0	0.6%	0.6%	1	0.0%	0.4%	0.0%	1787	CLTX	85	1787	CLTX	85
132	188	C8 PARAFFIN	1.5%	14.0	0.00%	0.0	1.5%	1.5%	1	0.0%	0.0%	0.3%	1240	D2CO	86	1240	D2CO	86
133	332	C12 AROMATIC	1.5%	13.9	0.00%	0.0	1.5%	1.5%	1	0.0%	0.0%	0.3%	2675	D2CO	86	2675	D2CO	86
134	330	C12 AROMATIC	1.9%	7.7	0.00%	0.0	1.9%	1.9%	1	0.5%	0.0%	0.0%	1852	DLTX	84	1852	DLTX	84
135	276	1,2-DIMETHYL-4-ETHYLBENZENE	1.4%	8.5	0.00%	0.0	1.4%	1.4%	1	0.0%	0.4%	0.0%	1655	DUNC	85	1655	DUNC	85
136	397	C8 PARAFFIN	3.1%	53.5	0.01%	0.1	3.1%	3.1%	1	0.5%	0.0%	0.0%	1423	FWTX	84	1423	FWTX	84
137	214	2,3-DIMETHYLHEPTANE	1.3%	22.9	0.00%	0.0	1.3%	1.3%	1	0.5%	0.0%	0.0%	1423	FWTX	84	1423	FWTX	84
138	111	Unknown	1.7%	8.0	0.00%	0.0	1.7%	1.7%	1	0.0%	0.0%	0.3%	2303	FWTX	86	2303	FWTX	86
139	190	C8 PARAFFIN	1.8%	19.9	0.00%	0.0	1.8%	1.8%	1	0.0%	0.4%	0.0%	1702	HITX	85	1702	HITX	85
140	266	1,3-DIETHYLBENZENE	1.7%	21.7	0.00%	0.0	1.7%	1.7%	1	0.5%	0.0%	0.0%	1218	ININ	84	1218	ININ	84
141	121	1-PENTENE	3.0%	19.2	0.00%	0.0	3.0%	3.0%	1	0.5%	0.0%	0.0%	1343	ININ	84	1343	ININ	84
142	284	1,2,4,5-TETRAMETHYLBENZENE	1.8%	26.4	0.00%	0.0	1.8%	1.8%	1	0.5%	0.0%	0.0%	1351	MTN	84	1351	MTN	84
143	400	C10 PARAFFIN	3.0%	21.2	0.00%	0.0	3.0%	3.0%	1	0.5%	0.0%	0.0%	1190	ORTX	84	1190	ORTX	84
144	302	C11 AROMATIC	1.0%	2.9	0.00%	0.0	1.0%	1.0%	1	0.0%	0.4%	0.0%	1335	ORTX	85	1335	ORTX	85
145	180	25DIMETHYLHEXANE,3MECYCLOHEXEN	1.1%	16.9	0.00%	0.0	1.1%	1.1%	1	0.0%	0.4%	0.0%	1029	P1PA	85	1029	P1PA	85
146	157	2,4-DIMETHYLPENTANE	4.8%	29.5	0.01%	0.0	4.8%	4.8%	1	0.0%	0.4%	0.0%	2296	PTNE	85	2296	PTNE	85
147	346	C7 OLEFIN	2.2%	3.9	0.00%	0.0	2.2%	2.2%	1	0.5%	0.0%	0.0%	1820	RVA	84	1820	RVA	84
148	293	C11 AROMATIC	1.5%	2.8	0.00%	0.0	1.5%	1.5%	1	0.5%	0.0%	0.0%	1820	RVA	84	1820	RVA	84
149	349	C8 OLEFIN	1.5%	8.6	0.00%	0.0	1.5%	1.5%	1	0.0%	0.4%	0.0%	1932	RVA	85	1932	RVA	85
150	197	C8 PARAFFIN	1.8%	6.5	0.00%	0.0	1.8%	1.8%	1	0.0%	0.4%	0.0%	1339	SLNO	85	1339	SLNO	85
151	133	2,2-DIMETHYLBUTANE	2.4%	26.0	0.00%	0.0	2.4%	2.4%	1	0.0%	0.4%	0.0%	2534	SLNO	85	2534	SLNO	85
152	286	C10 AROMATIC	1.2%	7.8	0.00%	0.0	1.2%	1.2%	1	0.5%	0.0%	0.0%	1244	SWPA	84	1244	SWPA	84
153	328	C13 PRAFFIN	2.2%	10.0	0.00%	0.0	2.2%	2.2%	1	0.5%	0.0%	0.0%	1285	SWPA	84	1285	SWPA	84
154	398	C9 PARAFFIN	2.5%	10.6	0.00%	0.0	2.5%	2.5%	1	0.5%	0.0%	0.0%	1439	SWPA	84	1439	SWPA	84
155	233	C10 PARAFFIN	2.0%	23.9	0.00%	0.0	2.0%	2.0%	1	0.5%	0.0%	0.0%	1344	TCTX	84	1344	TCTX	84
156	155	c&t-3-METHYL-2-PENTENE	0.9%	20.0	0.00%	0.0	0.9%	0.9%	1	0.5%	0.0%	0.0%	1483	TCTX	84	1483	TCTX	84
157	387	C7 OLEFIN	0.9%	19.3	0.00%	0.0	0.9%	0.9%	1	0.5%	0.0%	0.0%	1483	TCTX	84	1483	TCTX	84
158	348	C7 OLEFIN	0.8%	16.5	0.00%	0.0	0.8%	0.8%	1	0.5%	0.0%	0.0%	1483	TCTX	84	1483	TCTX	84
159	415	C7 OLEFIN	0.7%	15.8	0.00%	0.0	0.7%	0.7%	1	0.5%	0.0%	0.0%	1483	TCTX	84	1483	TCTX	84
160	178	c-HEPTENE-2	1.9%	14.5	0.00%	0.0	1.9%	1.9%	1	0.5%	0.0%	0.0%	1635	TCTX	84	1635	TCTX	84
161	122	C5 OLEFIN	1.7%	12.6	0.00%	0.0	1.7%	1.7%	1	0.0%	0.4%	0.0%	1122	TCTX	85	1122	TCTX	85
162	135	C6 OLEFIN	1.0%	2.2	0.00%	0.0	1.0%	1.0%	1	0.0%	0.4%	0.0%	2492	TCTX	85	2492	TCTX	85
163	334	C12 AROMATIC	4.8%	64.2	0.01%	0.1	4.8%	4.8%	1	0.5%	0.0%	0.0%	1220	UDC	84	1220	UDC	84
164	211	C9 PARAFFIN	1.3%	5.8	0.00%	0.0	1.3%	1.3%	1	0.5%	0.0%	0.0%	1360	UPFL	84	1360	UPFL	84
165	196	C8 PARAFFIN	1.8%	9.6	0.00%	0.0	1.8%	1.8%	1	0.5%	0.0%	0.0%	1705	UPFL	84	1705	UPFL	84

Basic Statistics

EPA GC Data

The master list of top 20 compounds based on the remaining 773 canisters comprises 165 species. Figure 3 shows the canister and city-year average carbon fraction accounted for by the top 20 in each canister sorted from highest to lowest. The maximum, average, and minimum NMOC in the 773 canisters was 2764 ppbC, 761 ppbC, and 175 ppbC. These values compare well with those reported by McAllisters.[12] Note that McAllister only analyzed 1985 data, but had a sample size of 1500. The McAllister statistics are shown below Figure 2 and his average was 755 ppbC. A plot of the total NMOC in each canister and the mean value for each city-year is shown in Figure 4. The order of city-years is the same as in Figure 3. A frequency distribution for NMOC concentration is shown in Figure 5. The plot shows a typical log-normal distribution, which, except for the extremes that have been trimmed, appears very similar to that shown in Figure 2.

Three city-years' "line chromatograms" for the top 20 compounds are shown in Figure 6, 7, and 8. Analysis of the data, to be shown below, indicate that these cities belong to different clusters of different HC composition. The x-axis on these plots is retention time (*i.e.*, unique to each HC species) and the y-axis is the relative carbon fraction in each canister. All canisters for a city-year are plotted on top of each other, and the symbols show the relative scatter for a given species. One can judge the consistency of the composition in each city-year from these plots. In addition, by overlaying the plots, you can estimate the city-to-city variation in the major species.

WSU Aloft GC Data

The average NMOC of the selected 53 canisters was 40 ppbC. Figure 9 shows the frequency distribution of aloft concentrations (including the aldehydes). The geometric mean concentration was 35 ppbC.

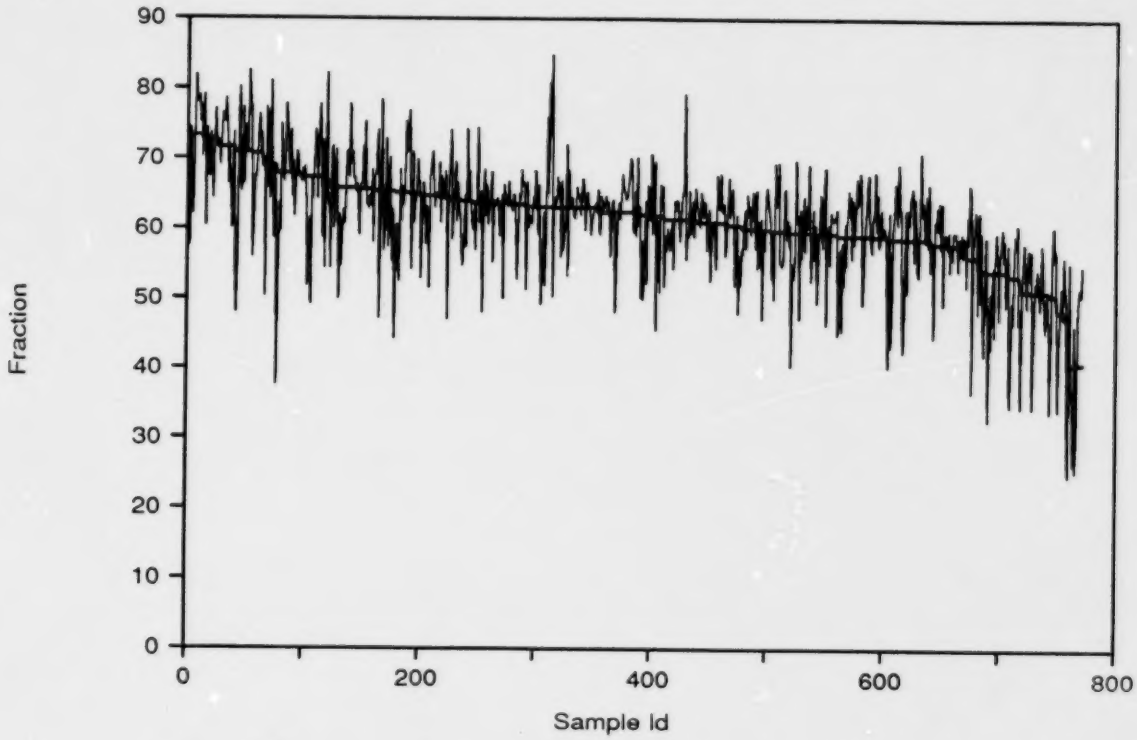

Figure 3. Canister and city-year average carbon fraction accounted for by the top 20 compounds in each canister sorted from highest to lowest.

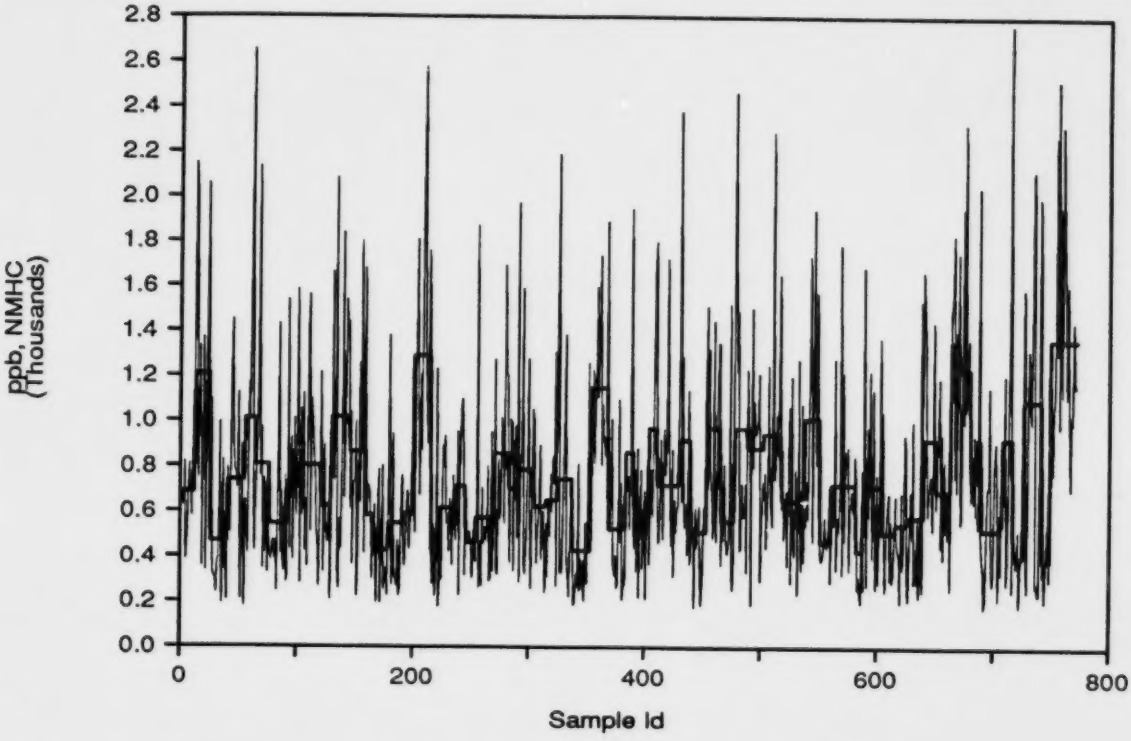

Figure 4. Total NMOC in each canister and the mean value for each city-year.

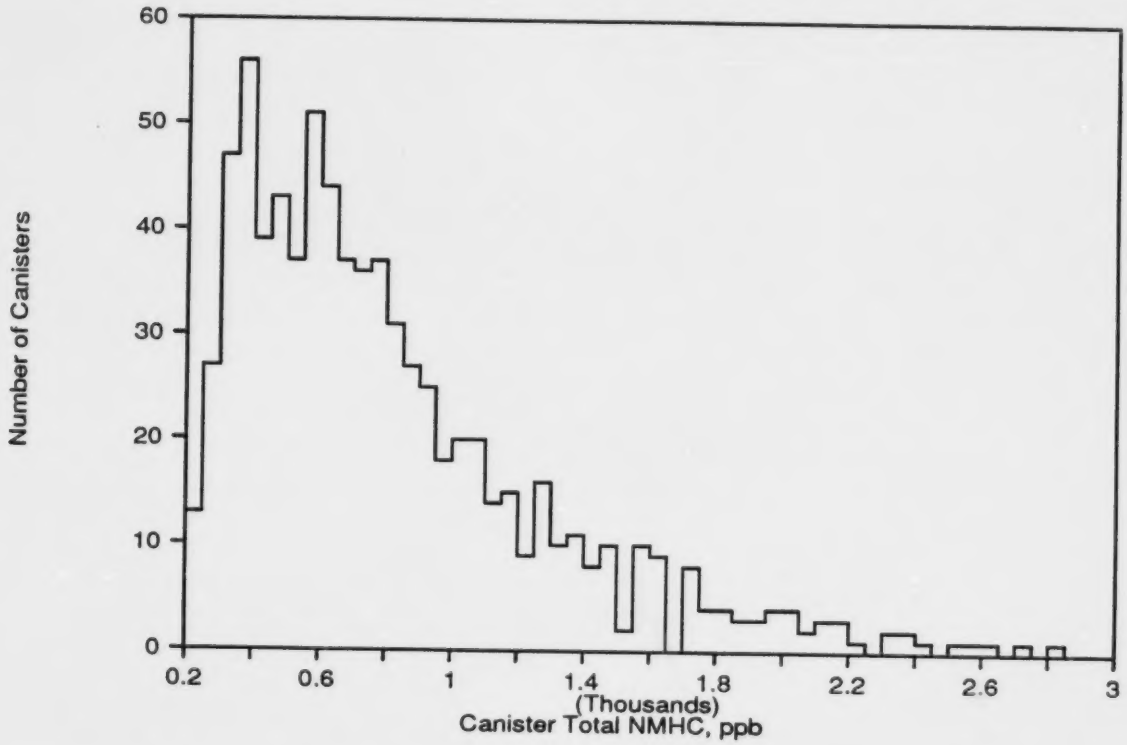

Figure 5. Frequency Distribution of Total NMOC Concentrations in Canisters for 1984, 1985, 1986.

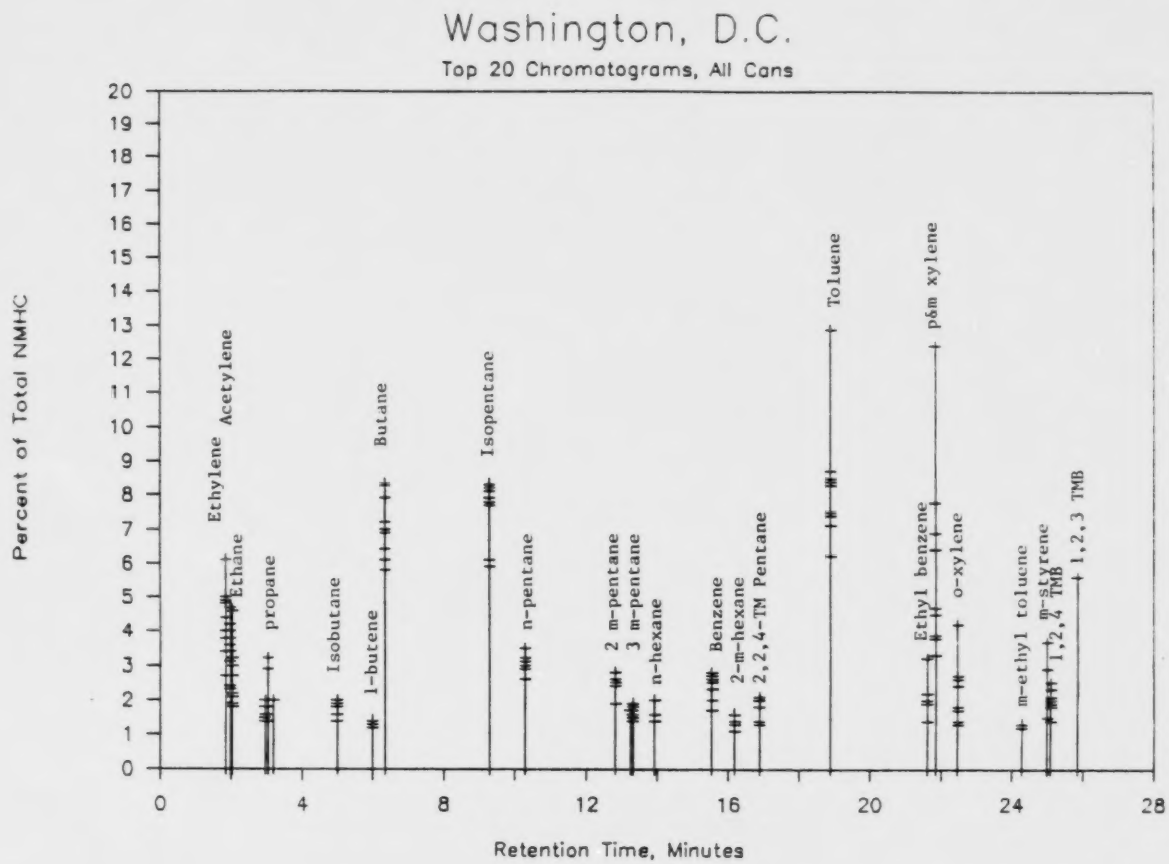

Figure 6. Line Chromatograms for Washington DC.

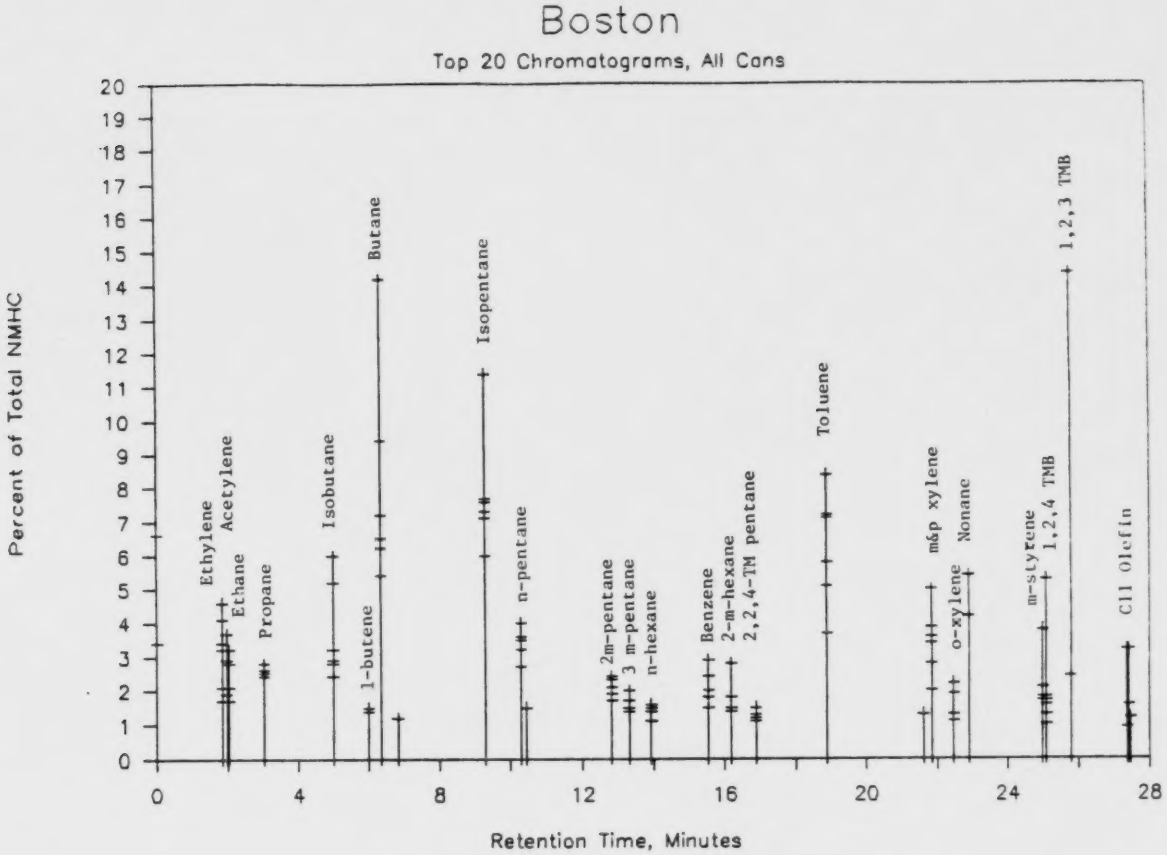

Figure 7. Line Chromatograms for Boston MA.

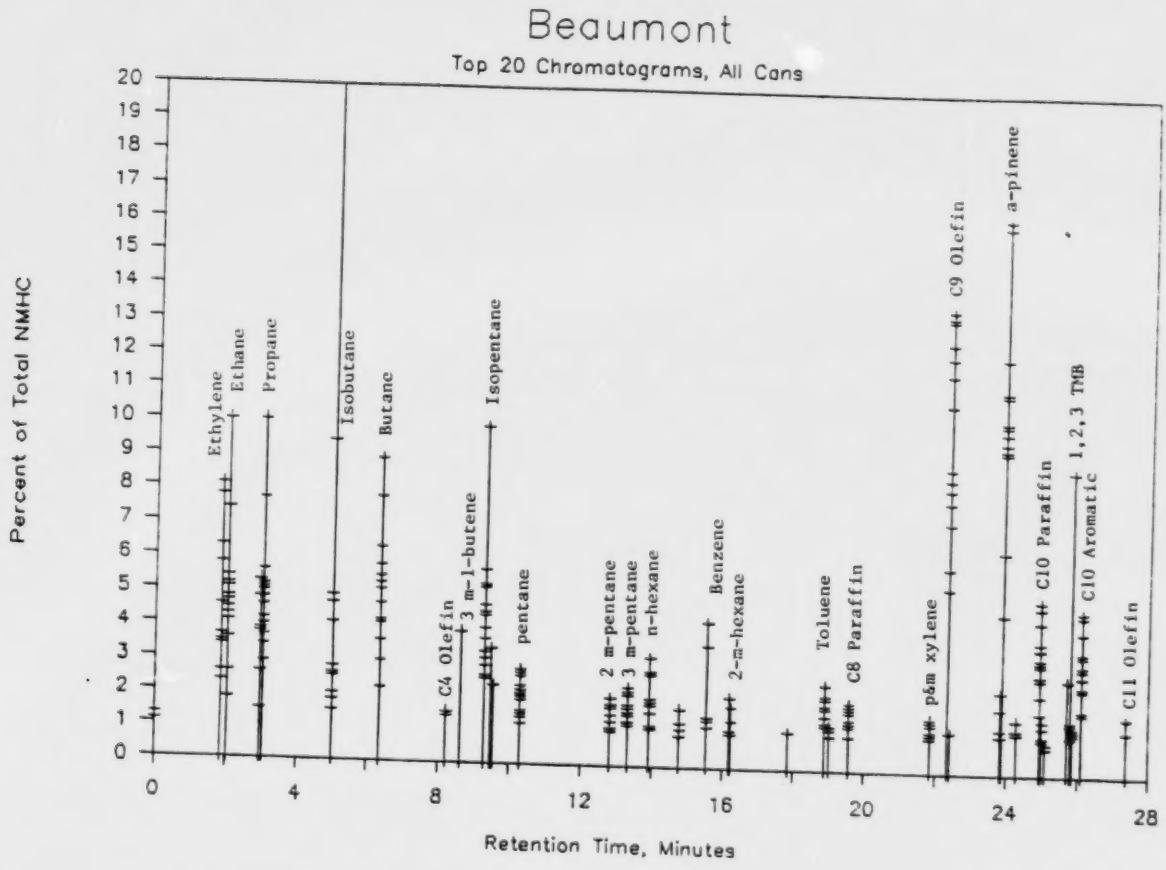

Figure 8. Line Chromatograms for Beaumont TX.

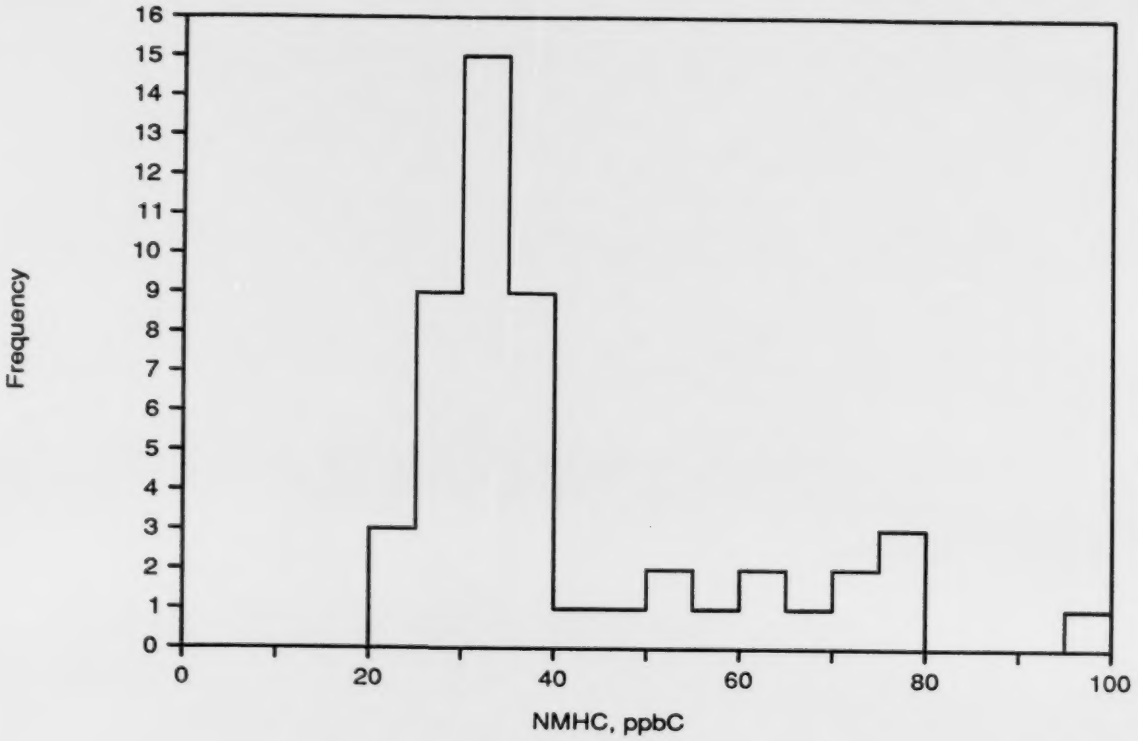

Figure 9. Frequency Distribution of Aloft Hydrocarbon Concentrations.

Speciation Database

The UNC hydrocarbon characteristics database was updated to include the guidance given by SAI[14] and by SAPRC/ERT.[2] A copy of this data base is included in the Appendix with the speciation processing program.

In the Carter, Atkinson, Lurmann Mechanism, molecules of a species in the urban HC mixture are assigned to a surrogate molecule in the mechanism. If the surrogate has more carbon than the mixture species, then carbon is gained; if the surrogate has fewer carbon atoms than the mixture species, then carbon will be lost. In the Carbon Bond Mechanisms, molecules in the urban HC mixture are broken up according to the type of bonding they have and the parts are assigned to species in the mechanism; all the carbons in the mixture molecule are assigned to model species and no carbon is gained or lost. To provide for comparison between the two mechanisms new species were added to the speciation for each mechanism.

The species UNK (unknown species) was added to both mechanisms to account for those compounds in the canisters that did not have a species identification. The species MISS was added to the CAL mechanism to account for the carbon difference between the species in the canister and the species it was assigned to in the mechanism. Thus, when a C_{11} alkane was assigned to ALK7, which has a carbon number of 7, 4 carbons were also assigned to MISS thus preserving the total carbon concentration in this mechanism. Additional calculations were done to speciate the MISS fraction (*i.e.*, to show the origin of the carbon assigned to MISS).

Finally, the canister data contained classified, but *unidentified* species, for example "C_{11} olefin" or "C_{12} aromatic." The carbon numbers for these unidentified species ranged from 3 to 13 for the alkane species, from 4 to 11 for the olefin species, and from 9 to 12 for the aromatic species. The alkane species could be readily assigned to a mechanism species; olefin and aromatic species were more difficult. For these, each compound was treated by specific rules based on class and carbon number. For example,

1) all olefins were assumed to be terminal;
2) C_9 and C_{10} aromatics were assumed to be 50% mono- , 35% di- and 15% tri-substituted;
3) C_{11} and C_{12} aromatics were assumed to be 50% di- and 50% tri- substituted.

Speciation Operation

In calculating the composition from multiple canisters, the calculations were done as if each canister were added to a well mixed bag and the bag composition were

then determined. All carbon mass was conserved and thus the concentration of a canister determined how much it contributed to the final bag composition.

Results

Fraction Speciated to Mechanisms Species

Tables 4a, b, and c list the carbon fraction for each mechanism species for all 66 city-years. For reasons given below, the ordering of city-years in this table is divided into four groups. In the first part of the discussion, we will ignore this grouping, and later we will explain the groups. In Table 4, the third column is the sum of the individual species mixing ratio in the canister (*i.e.*, the total NMOC) in units of ppbC. The fourth and fifth columns are the sum of the individual species treated by CB4 or CAL lumping. Some of these latter values are not quite equal to the NMOC because of the presence of the sub-ppbC wrongly-identified species in the canisters (*i.e.*, a nonexistent species id number was assigned to the species and thus it could not be classified). Figure 10 shows the CB4 total NMOC and CAL total NMOC plotted against the canister NMOC. The fraction carbon accounted for in each canister by each mechanism's species was almost always greater than 99%.

Tables 5a and b give the computed aloft carbon fractions for both mechanisms. Table 6 gives the computed carbon fractions for the UNC autoexhaust analyses.

Table 4. Carbon Fractions for Each Mechanism Species for All 66 City-years.

CLUSTER 1 CB4

City	Yr	Sam#	NMHC	CBTOT	CLTOT	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR
WDC	85	9	589	589	589	0.533	0.045	0.037	0.022	0.122	0.162	0.070	0.008	0.001
BPCT	86	16	429	429	427	0.533	0.048	0.036	0.027	0.114	0.163	0.075	0.005	0.000
TRNJ	86	15	947	947	945	0.517	0.043	0.038	0.023	0.123	0.157	0.078	0.020	0.000
BHAL	84	4	921	921	913	0.527	0.039	0.033	0.018	0.105	0.172	0.093	0.011	0.003
RVA	84	9	401	401	400	0.550	0.032	0.040	0.018	0.141	0.137	0.059	0.014	0.009
ALL		53	635	635	633	0.527	0.043	0.037	0.023	0.121	0.159	0.076	0.013	0.001

CLUSTER 2,4,7

City	Yr	Sam#	NMHC	CBTOT	CLTOT	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR
DLTX	86	13	561	561	559	0.535	0.037	0.028	0.026	0.109	0.152	0.098	0.015	0.000
ELTX	86	10	703	703	702	0.576	0.044	0.033	0.020	0.090	0.129	0.105	0.002	0.000
CLOH	85	16	1019	1019	1016	0.584	0.036	0.025	0.017	0.090	0.134	0.105	0.008	0.001
P1PA	85	11	788	788	786	0.585	0.028	0.035	0.020	0.099	0.130	0.082	0.019	0.001
CLTX	84	8	462	461	460	0.555	0.069	0.034	0.012	0.084	0.109	0.114	0.020	0.003
S2UT	86	13	859	859	858	0.599	0.043	0.030	0.022	0.094	0.121	0.088	0.004	0.000
ELTX	85	13	790	790	789	0.593	0.036	0.031	0.019	0.087	0.115	0.104	0.014	0.001
BHAL	86	13	745	745	744	0.581	0.035	0.034	0.023	0.090	0.146	0.087	0.004	0.000
PHPA	84	7	865	865	859	0.570	0.084	0.032	0.020	0.097	0.114	0.074	0.006	0.002
ELTX	84	7	968	968	966	0.594	0.032	0.034	0.030	0.092	0.105	0.078	0.031	0.003
FWTX	85	19	719	719	718	0.586	0.037	0.042	0.025	0.092	0.124	0.083	0.010	0.002
H2TX	86	12	973	973	971	0.582	0.038	0.032	0.036	0.091	0.139	0.079	0.004	0.000
FWTX	84	13	1013	1013	1012	0.593	0.036	0.034	0.022	0.094	0.119	0.088	0.013	0.002
AKOH	84	10	465	465	464	0.563	0.028	0.039	0.019	0.102	0.124	0.114	0.007	0.005
DLTX	85	21	723	723	721	0.592	0.032	0.033	0.025	0.096	0.129	0.082	0.011	0.001
SWPA	84	10	546	546	545	0.587	0.050	0.033	0.020	0.097	0.116	0.077	0.017	0.003
ININ	84	10	920	920	916	0.587	0.040	0.030	0.017	0.112	0.134	0.074	0.003	0.004
C2IL	86	14	885	885	882	0.592	0.037	0.031	0.020	0.109	0.140	0.063	0.010	0.000
MIFL	84	3	658	658	657	0.595	0.031	0.022	0.019	0.118	0.151	0.049	0.011	0.004
BONA	85	6	425	425	424	0.596	0.026	0.029	0.029	0.092	0.147	0.059	0.021	0.002
RVA	85	12	507	507	506	0.588	0.036	0.035	0.023	0.104	0.128	0.064	0.020	0.002
WDC	84	10	924	924	922	0.580	0.040	0.039	0.024	0.114	0.141	0.053	0.006	0.003
DLTX	84	13	695	695	694	0.577	0.030	0.031	0.022	0.105	0.135	0.074	0.024	0.003
CNOH	84	5	736	736	735	0.602	0.031	0.035	0.022	0.102	0.138	0.057	0.010	0.003
CHNC	84	15	524	524	523	0.575	0.039	0.044	0.023	0.108	0.138	0.055	0.017	0.003
DUNC	85	3	546	546	545	0.550	0.042	0.052	0.025	0.098	0.154	0.055	0.022	0.002
ATGA	84	9	922	922	921	0.591	0.039	0.038	0.023	0.108	0.142	0.053	0.004	0.002
RLNC	85	16	1093	1093	1092	0.556	0.053	0.045	0.030	0.097	0.153	0.059	0.006	0.000
WPFL	84	7	385	385	384	0.579	0.031	0.036	0.016	0.123	0.149	0.048	0.011	0.007
CHTN	84	9	1363	1363	1361	0.576	0.031	0.030	0.018	0.119	0.158	0.059	0.007	0.002
WDC	86	8	429	429	428	0.564	0.032	0.026	0.017	0.113	0.157	0.084	0.007	0.000
FWTX	86	16	574	574	573	0.584	0.035	0.030	0.025	0.101	0.144	0.075	0.005	0.000
P2PA	85	8	701	701	699	0.580	0.035	0.035	0.022	0.112	0.132	0.074	0.009	0.001
BLMO	86	10	651	651	649	0.553	0.035	0.035	0.025	0.113	0.148	0.082	0.009	0.000
D2CO	86	15	1149	1149	1148	0.555	0.040	0.031	0.024	0.132	0.138	0.078	0.003	0.000
KCMO	85	15	526	525	525	0.562	0.040	0.030	0.017	0.106	0.140	0.095	0.010	0.001
ATGA	86	14	513	513	512	0.566	0.042	0.033	0.024	0.106	0.151	0.073	0.004	0.000
HNY	86	12	561	561	559	0.576	0.037	0.030	0.027	0.107	0.140	0.076	0.006	0.000
SLMO	85	17	651	651	648	0.574	0.029	0.028	0.017	0.109	0.136	0.093	0.014	0.001
BHY	86	16	717	717	715	0.567	0.034	0.032	0.029	0.116	0.151	0.065	0.005	0.000
WHCT	86	15	578	578	573	0.554	0.036	0.038	0.031	0.118	0.145	0.070	0.008	0.000
HTN	84	7	1353	1353	1351	0.565	0.042	0.041	0.032	0.109	0.143	0.060	0.007	0.001
C1IL	86	10	1233	1233	1229	0.579	0.037	0.029	0.021	0.124	0.140	0.060	0.009	0.000
ALL		491	757	757	756	0.577	0.038	0.033	0.023	0.104	0.137	0.077	0.010	0.001

Table 4. (cont.)

CLUSTER 3,6 CB4

City	Yr	Sam#	NMHC	CBTOT	CLTOT	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR
BMTX	86	12	688	687	687	0.625	0.091	0.032	0.015	0.046	0.066	0.120	0.004	0.000
LCLA	85	15	740	740	739	0.601	0.024	0.023	0.013	0.054	0.087	0.184	0.015	0.001
TCTX	84	12	808	808	808	0.597	0.024	0.030	0.016	0.054	0.063	0.188	0.025	0.003
BRLA	85	14	547	547	546	0.612	0.037	0.036	0.018	0.073	0.093	0.118	0.011	0.001
H1TX	85	20	806	806	805	0.590	0.035	0.062	0.023	0.072	0.086	0.123	0.008	0.001
ORTX	84	7	583	583	581	0.602	0.051	0.026	0.012	0.076	0.082	0.135	0.012	0.004
ORTX	85	12	616	616	614	0.590	0.046	0.053	0.018	0.054	0.077	0.140	0.020	0.002
H1TX	86	13	1205	1205	1204	0.662	0.027	0.034	0.025	0.060	0.084	0.103	0.004	0.000
TLOK	86	15	470	470	469	0.646	0.026	0.029	0.014	0.055	0.088	0.120	0.021	0.000
BMTX	84	9	1013	1013	1012	0.670	0.038	0.025	0.021	0.046	0.061	0.125	0.014	0.001
S1UT	86	15	1289	1289	1288	0.652	0.024	0.045	0.027	0.064	0.082	0.099	0.007	0.000
BMTX	85	14	1360	1360	1356	0.633	0.036	0.063	0.037	0.052	0.085	0.077	0.015	0.001
ALL		158	851	851	850	0.627	0.035	0.042	0.023	0.059	0.080	0.121	0.012	0.001

CLUSTER 8

City	Yr	Sam#	NMHC	CBTOT	CLTOT	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR
PTNE	85	10	624	624	619	0.648	0.023	0.034	0.035	0.085	0.098	0.066	0.009	0.001
D1CO	86	14	866	866	858	0.609	0.035	0.029	0.025	0.086	0.115	0.097	0.004	0.000
PHPA	86	12	429	429	424	0.621	0.027	0.029	0.017	0.093	0.116	0.085	0.011	0.000
TCTX	85	13	549	549	543	0.616	0.034	0.039	0.022	0.073	0.101	0.104	0.009	0.002
KCMO	84	11	973	973	967	0.621	0.031	0.030	0.018	0.102	0.115	0.076	0.004	0.002
ALL		60	690	689	687	0.621	0.031	0.032	0.023	0.089	0.110	0.087	0.007	0.001

NOT INCLUDED IN ANY OTHER CLUSTER

CLTX	85	11	623	623	621	0.482	0.164	0.061	0.013	0.064	0.082	0.105	0.028	0.001

Cluster Averages Repeated Here!

	Sam#	NMHC	CBTOT	CLTOT	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR
Ave 1	53	635	635	633	0.527	0.043	0.037	0.023	0.121	0.159	0.076	0.013	0.001
Ave 2,4,	491	757	757	756	0.577	0.038	0.033	0.023	0.104	0.137	0.077	0.010	0.001
Ave 3,6	158	851	851	850	0.627	0.035	0.042	0.023	0.059	0.080	0.121	0.012	0.001
Ave 8	60	690	689	687	0.621	0.031	0.032	0.023	0.089	0.110	0.087	0.007	0.001

City	Yr	Sam#	NMHC	CBTOT	CLTOT	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR
ALL	ALL	773	761	761	759	0.588	0.039	0.036	0.023	0.093	0.122	0.088	0.010	0.001

Table 4. (cont.)

CLUSTER 1 CAL

City	Yr	Sam#	NMHC	CBTOT	CLTOT	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK
WDC	85	9	589	589	589	0.189	0.267	0.045	0.048	0.030	0.113	0.122	0.041	0.000	0.000	0.000	0.099	0.038	0.008
BPCT	86	16	429	429	427	0.184	0.266	0.048	0.048	0.033	0.106	0.116	0.055	0.000	0.000	0.000	0.098	0.040	0.005
TRNJ	86	15	947	947	945	0.180	0.253	0.043	0.054	0.027	0.120	0.109	0.052	0.000	0.000	0.000	0.104	0.038	0.020
BHAL	84	4	921	921	913	0.139	0.309	0.039	0.053	0.024	0.082	0.113	0.064	0.000	0.000	0.000	0.130	0.035	0.011
RVA	84	9	401	401	400	0.160	0.280	0.032	0.069	0.030	0.077	0.083	0.058	0.000	0.000	0.000	0.166	0.030	0.014
ALL		53	635	635	633	0.176	0.267	0.043	0.053	0.029	0.107	0.110	0.053	0.000	0.000	0.000	0.111	0.037	0.013

CLUSTER 2,4,7

City	Yr	Sam#	NMHC	CBTOT	CLTOT	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK
DLTX	86	13	561	561	559	0.188	0.273	0.037	0.036	0.032	0.103	0.100	0.059	0.000	0.000	0.000	0.105	0.052	0.015
ELTX	86	10	703	703	702	0.205	0.324	0.044	0.047	0.024	0.087	0.090	0.042	0.000	0.000	0.000	0.085	0.050	0.002
CLOH	85	16	1019	1019	1016	0.256	0.272	0.036	0.037	0.021	0.082	0.087	0.050	0.000	0.000	0.000	0.098	0.053	0.008
P1PA	85	11	788	788	786	0.250	0.273	0.028	0.044	0.030	0.090	0.083	0.050	0.000	0.000	0.000	0.095	0.038	0.019
CLTX	84	8	462	461	460	0.218	0.270	0.069	0.055	0.019	0.064	0.070	0.041	0.000	0.000	0.000	0.117	0.056	0.020
S2UT	86	13	859	859	858	0.185	0.352	0.043	0.042	0.027	0.091	0.086	0.037	0.000	0.000	0.000	0.087	0.045	0.004
ELTX	85	13	790	790	789	0.222	0.316	0.036	0.045	0.024	0.078	0.079	0.038	0.000	0.000	0.000	0.095	0.052	0.014
BHAL	86	13	745	745	744	0.228	0.282	0.035	0.043	0.032	0.084	0.100	0.051	0.000	0.000	0.000	0.099	0.041	0.004
PHPA	84	7	865	865	859	0.220	0.294	0.085	0.052	0.024	0.080	0.075	0.042	0.000	0.000	0.000	0.089	0.033	0.006
ELTX	84	7	968	968	966	0.239	0.294	0.032	0.055	0.034	0.072	0.071	0.036	0.000	0.000	0.000	0.095	0.039	0.031
FWTX	85	19	719	719	718	0.200	0.311	0.037	0.057	0.035	0.078	0.084	0.043	0.000	0.000	0.000	0.102	0.043	0.010
H2TX	86	12	973	973	971	0.218	0.287	0.038	0.044	0.041	0.086	0.093	0.051	0.000	0.000	0.000	0.099	0.039	0.004
FWTX	84	13	1013	1013	1012	0.194	0.321	0.036	0.052	0.028	0.075	0.080	0.041	0.000	0.000	0.000	0.114	0.046	0.013
AXCH	84	10	465	465	464	0.206	0.269	0.029	0.050	0.036	0.066	0.077	0.050	0.000	0.000	0.000	0.149	0.062	0.007
DLTX	85	21	723	723	721	0.195	0.326	0.032	0.045	0.033	0.088	0.083	0.050	0.000	0.000	0.000	0.095	0.044	0.011
SWPA	84	10	546	546	545	0.208	0.304	0.049	0.053	0.027	0.075	0.075	0.044	0.000	0.000	0.000	0.112	0.036	0.017
ININ	84	10	920	920	916	0.195	0.322	0.040	0.052	0.022	0.086	0.088	0.049	0.000	0.000	0.000	0.109	0.034	0.003
C2IL	86	14	885	885	882	0.213	0.306	0.037	0.043	0.023	0.103	0.096	0.050	0.000	0.000	0.000	0.088	0.031	0.010
MIFL	84	3	658	658	657	0.186	0.335	0.031	0.040	0.023	0.091	0.096	0.058	0.000	0.000	0.000	0.101	0.028	0.011
BOMA	85	6	425	425	424	0.261	0.267	0.026	0.041	0.035	0.078	0.075	0.080	0.000	0.000	0.000	0.087	0.029	0.021
RVA	85	12	507	507	506	0.222	0.290	0.036	0.047	0.032	0.089	0.078	0.055	0.000	0.000	0.000	0.097	0.034	0.020
WDC	84	10	924	924	922	0.181	0.311	0.040	0.058	0.032	0.093	0.092	0.052	0.000	0.000	0.000	0.107	0.028	0.006
DLTX	84	13	695	695	694	0.184	0.318	0.030	0.047	0.029	0.084	0.090	0.047	0.000	0.000	0.000	0.109	0.038	0.024
CNOH	84	5	736	736	735	0.202	0.305	0.031	0.054	0.028	0.077	0.087	0.055	0.000	0.000	0.000	0.123	0.029	0.010
CHNC	84	15	524	524	523	0.167	0.311	0.039	0.056	0.037	0.084	0.091	0.050	0.000	0.000	0.000	0.121	0.028	0.017
DUNC	85	3	546	546	545	0.161	0.304	0.042	0.048	0.049	0.084	0.101	0.058	0.000	0.000	0.000	0.100	0.030	0.023
ATGA	84	9	922	922	921	0.148	0.351	0.039	0.055	0.030	0.092	0.094	0.051	0.000	0.000	0.000	0.109	0.029	0.004
RLNC	85	16	1093	1093	1092	0.161	0.307	0.053	0.050	0.046	0.092	0.103	0.053	0.000	0.000	0.000	0.100	0.030	0.006
WPFL	84	7	385	385	384	0.159	0.316	0.031	0.068	0.022	0.070	0.092	0.062	0.000	0.000	0.000	0.148	0.023	0.011
CHTN	84	9	1363	1363	1361	0.137	0.335	0.031	0.042	0.025	0.105	0.106	0.055	0.000	0.000	0.000	0.125	0.031	0.007
WDC	86	8	429	429	428	0.229	0.269	0.032	0.034	0.022	0.109	0.107	0.055	0.000	0.000	0.000	0.092	0.043	0.007
FWTX	86	16	574	574	573	0.213	0.309	0.035	0.041	0.031	0.096	0.100	0.049	0.000	0.000	0.000	0.083	0.038	0.005
P2PA	85	8	701	701	699	0.235	0.286	0.035	0.050	0.027	0.102	0.085	0.050	0.000	0.000	0.000	0.085	0.035	0.009
BLMD	86	10	651	651	649	0.213	0.265	0.035	0.046	0.032	0.108	0.102	0.051	0.000	0.000	0.000	0.097	0.042	0.009
D2CO	86	15	1149	1149	1148	0.154	0.325	0.040	0.044	0.030	0.127	0.099	0.043	0.000	0.000	0.000	0.094	0.042	0.003
KCMO	85	15	526	525	525	0.190	0.292	0.040	0.042	0.022	0.096	0.081	0.065	0.000	0.000	0.000	0.108	0.053	0.010
ATGA	86	14	513	513	512	0.201	0.291	0.042	0.042	0.032	0.101	0.104	0.052	0.000	0.000	0.000	0.094	0.038	0.004
HNY	86	12	561	561	559	0.224	0.272	0.037	0.042	0.030	0.102	0.095	0.051	0.000	0.000	0.000	0.099	0.040	0.006
SLMO	85	17	651	651	648	0.222	0.294	0.029	0.039	0.022	0.100	0.087	0.053	0.000	0.000	0.000	0.100	0.040	0.014
BNY	86	16	717	717	715	0.212	0.270	0.034	0.044	0.034	0.111	0.102	0.055	0.000	0.000	0.000	0.100	0.034	0.005
NHCT	86	15	578	578	573	0.184	0.283	0.036	0.052	0.041	0.112	0.103	0.049	0.000	0.000	0.000	0.100	0.032	0.008
HTN	84	7	1353	1353	1351	0.155	0.320	0.042	0.056	0.041	0.099	0.097	0.049	0.000	0.000	0.000	0.103	0.032	0.007
C1IL	86	10	1233	1233	1229	0.179	0.315	0.037	0.041	0.026	0.119	0.094	0.052	0.000	0.000	0.000	0.098	0.031	0.009
ALL		491	757	757	756	0.198	0.304	0.038	0.047	0.030	0.093	0.091	0.049	0.000	0.000	0.000	0.101	0.039	0.010

Table 4. (cont.)

CLUSTER 3,6 CAL

City	Yr	Sam#	NMHC	CBTOT	CLTOT	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK
BMTX	86	12	688	687	687	0.331	0.248	0.091	0.054	0.020	0.042	0.047	0.023	0.000	0.000	0.000	0.083	0.057	0.004
LCLA	85	15	740	740	739	0.340	0.237	0.023	0.032	0.019	0.045	0.051	0.039	0.000	0.000	0.000	0.106	0.092	0.015
TCTX	84	12	808	808	808	0.301	0.251	0.024	0.049	0.021	0.035	0.039	0.025	0.000	0.000	0.000	0.134	0.095	0.025
BRLA	85	14	547	547	546	0.277	0.282	0.037	0.052	0.023	0.064	0.065	0.030	0.000	0.000	0.000	0.096	0.063	0.011
HITX	85	20	806	806	805	0.259	0.250	0.035	0.085	0.035	0.067	0.059	0.029	0.000	0.000	0.000	0.110	0.063	0.008
ORTX	84	7	583	583	581	0.266	0.278	0.051	0.048	0.020	0.049	0.052	0.032	0.000	0.000	0.000	0.127	0.066	0.012
ORTX	85	12	616	616	614	0.296	0.239	0.046	0.055	0.047	0.039	0.050	0.031	0.000	0.000	0.000	0.108	0.069	0.020
HITX	86	13	1205	1205	1204	0.373	0.268	0.027	0.044	0.034	0.056	0.059	0.029	0.000	0.000	0.000	0.059	0.047	0.004
TLOK	86	15	470	470	469	0.341	0.284	0.026	0.041	0.019	0.052	0.057	0.035	0.000	0.000	0.000	0.065	0.058	0.021
BMTX	84	9	1013	1013	1012	0.353	0.306	0.038	0.038	0.026	0.039	0.040	0.022	0.000	0.000	0.000	0.063	0.061	0.014
SIUT	86	15	1289	1289	1288	0.300	0.313	0.024	0.066	0.032	0.061	0.058	0.027	0.000	0.000	0.000	0.071	0.042	0.007
BMTX	85	14	1360	1360	1356	0.204	0.230	0.037	0.077	0.054	0.043	0.056	0.031	0.000	0.000	0.000	0.218	0.036	0.015
ALL		158	851	851	850	0.298	0.265	0.035	0.057	0.032	0.051	0.054	0.029	0.000	0.000	0.000	0.108	0.059	0.012

CLUSTER 8

City	Yr	Sam#	NMHC	CBTOT	CLTOT	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK
PTNE	85	10	624	624	623	0.327	0.272	0.023	0.044	0.043	0.076	0.071	0.029	0.000	0.000	0.000	0.075	0.030	0.009
DICO	86	14	866	866	863	0.218	0.334	0.035	0.041	0.030	0.082	0.084	0.035	0.000	0.000	0.000	0.084	0.052	0.004
PHPA	86	12	429	429	427	0.302	0.281	0.027	0.043	0.023	0.085	0.085	0.037	0.000	0.000	0.000	0.065	0.040	0.011
TCTX	85	13	549	549	548	0.274	0.297	0.034	0.059	0.028	0.062	0.047	0.061	0.000	0.000	0.000	0.087	0.044	0.009
KCMO	84	11	973	973	971	0.190	0.350	0.031	0.049	0.023	0.084	0.077	0.040	0.000	0.000	0.000	0.110	0.041	0.004
ALL		60	690	689	687	0.248	0.316	0.031	0.047	0.029	0.078	0.074	0.040	0.000	0.000	0.000	0.088	0.043	0.007

NOT INCLUDED IN ANY OTHER CLUSTER

CLTX	85	11	623	623	621	0.139	0.198	0.164	0.110	0.020	0.055	0.051	0.033	0.000	0.000	0.000	0.146	0.055	0.028

Cluster Averages Repeated Here

	Sam#	NMHC	CBTOT	CLTOT	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK
Ave 1	53	635	635	633	0.176	0.267	0.043	0.053	0.029	0.107	0.110	0.053	0.000	0.000	0.000	0.111	0.037	0.013
Ave 2,4,	491	757	757	756	0.198	0.304	0.038	0.047	0.030	0.093	0.091	0.049	0.000	0.000	0.000	0.101	0.039	0.010
Ave 3,6	158	851	851	850	0.298	0.265	0.035	0.057	0.032	0.051	0.054	0.029	0.000	0.000	0.000	0.108	0.059	0.012
Ave 8	60	690	689	687	0.248	0.316	0.031	0.047	0.029	0.078	0.074	0.040	0.000	0.000	0.000	0.088	0.043	0.007

City	Yr	Sam#	NMHC	CBTOT	CLTOT	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK
ALL	ALL	773	761	761	759	0.223	0.292	0.039	0.050	0.030	0.083	0.082	0.044	0.000	0.000	0.000	0.103	0.044	0.010

Table 4. (cont.)

CLUSTER 1 CAL_MISSING

City	Yr	Sam#	NMHC	CBTOT	CLTOT	MPRPE	MTBUT	MALK4	MALK7	MTOL	MXYL	MTMB	MNR
WDC	85	9	589	589	589 |	0.032	0.008	-0.002	-0.004	0.006	0.014	0.004	0.041
BPCT	86	16	429	429	427 |	0.025	0.008	-0.001	-0.004	0.005	0.018	0.003	0.044
TRNJ	86	15	947	947	945 |	0.026	0.006	-0.002	0.011	0.008	0.015	0.004	0.037
BHAL	84	4	921	921	913 |	0.046	0.007	-0.001	-0.005	0.007	0.019	0.010	0.046
RVA	84	9	401	401	400 |	0.094	0.011	-0.002	0.003	0.006	0.015	0.008	0.031
ALL		53	635	635	633 |	0.036	0.007	-0.002	0.003	0.007	0.016	0.005	0.040

CLUSTER 2,4,7

City	Yr	Sam#	NMHC	CBTOT	CLTOT	MPRPE	MTBUT	MALK4	MALK7	MTOL	MXYL	MTMB	MNR
DLTX	86	13	561	561	559 |	0.021	0.011	0.000	-0.005	0.007	0.015	0.005	0.051
ELTX	86	10	703	703	702 |	0.021	0.005	0.001	-0.009	0.005	0.012	0.003	0.048
CLOH	85	16	1019	1019	1016 |	0.025	0.005	-0.005	-0.005	0.006	0.012	0.005	0.054
P1PA	85	11	788	788	786 |	0.029	0.014	-0.004	-0.004	0.007	0.012	0.005	0.035
CLTX	84	8	462	461	460 |	0.047	0.005	-0.002	-0.007	0.005	0.012	0.006	0.051
S2UT	86	13	859	859	858 |	0.024	0.006	0.000	-0.007	0.004	0.010	0.002	0.049
ELTX	85	13	790	790	789 |	0.032	0.006	-0.002	-0.009	0.005	0.010	0.003	0.049
BHAL	86	13	745	745	744 |	0.024	0.009	-0.005	0.000	0.006	0.015	0.004	0.046
PHPA	84	7	865	865	859 |	0.043	0.006	-0.002	-0.009	0.005	0.012	0.005	0.029
ELTX	84	7	968	968	966 |	0.049	0.006	-0.005	-0.012	0.005	0.010	0.004	0.038
FWTX	85	19	719	719	718 |	0.040	0.010	-0.001	-0.012	0.005	0.013	0.004	0.043
N2TX	86	12	973	973	971 |	0.026	0.011	-0.001	-0.003	0.007	0.014	0.004	0.040
FWTX	84	13	1013	1013	1012 |	0.049	0.008	-0.002	-0.010	0.006	0.012	0.005	0.046
AKOH	84	10	465	465	464 |	0.063	0.007	-0.004	-0.002	0.006	0.013	0.006	0.059
DLTX	85	21	723	723	721 |	0.033	0.010	-0.001	-0.012	0.005	0.012	0.004	0.044
SWPA	84	10	546	546	545 |	0.057	0.007	-0.001	-0.008	0.005	0.012	0.006	0.033
ININ	84	10	920	920	916 |	0.049	0.005	-0.001	-0.007	0.007	0.014	0.007	0.036
C2IL	86	14	885	885	882 |	0.025	0.007	-0.004	0.001	0.007	0.015	0.004	0.034
MIFL	84	3	658	658	657 |	0.049	0.005	0.001	-0.014	0.006	0.016	0.008	0.029
BOMA	85	6	425	425	424 |	0.036	0.008	-0.008	0.002	0.004	0.011	0.004	0.031
RVA	85	12	507	507	506 |	0.042	0.009	-0.005	-0.006	0.005	0.012	0.004	0.036
WDC	84	10	924	924	922 |	0.049	0.007	-0.003	-0.008	0.006	0.015	0.007	0.032
DLTX	84	13	695	695	694 |	0.047	0.008	-0.001	-0.008	0.007	0.013	0.006	0.037
CNOH	84	5	736	736	735 |	0.058	0.006	-0.003	0.000	0.008	0.015	0.008	0.031
CHNC	84	15	524	524	523 |	0.056	0.014	-0.001	-0.005	0.007	0.014	0.006	0.031
DUNC	85	3	546	546	545 |	0.034	0.013	0.001	-0.013	0.005	0.018	0.009	0.033
ATGA	84	9	922	922	921 |	0.047	0.008	-0.001	-0.004	0.006	0.015	0.007	0.032
RLNC	85	16	1093	1093	1092 |	0.029	0.017	-0.001	-0.007	0.006	0.014	0.005	0.036
WPFL	84	7	385	385	384 |	0.088	0.007	0.001	-0.003	0.006	0.018	0.009	0.022
CHTN	84	9	1363	1363	1361 |	0.040	0.006	-0.001	0.010	0.013	0.018	0.007	0.033
WDC	86	8	429	429	428 |	0.019	0.006	-0.004	0.002	0.006	0.014	0.004	0.045
FWTX	86	16	574	574	573 |	0.024	0.009	-0.001	-0.015	0.006	0.015	0.004	0.040
P2PA	85	8	701	701	699 |	0.032	0.006	-0.004	-0.007	0.007	0.011	0.003	0.036
BLND	86	10	651	651	649 |	0.025	0.008	-0.004	-0.004	0.006	0.015	0.004	0.046
D2CO	86	15	1149	1149	1148 |	0.026	0.008	0.000	-0.008	0.005	0.014	0.003	0.045
KCMO	85	15	526	525	525 |	0.030	0.006	0.001	-0.003	0.005	0.011	0.003	0.054
ATGA	86	14	513	513	512 |	0.023	0.010	-0.003	-0.004	0.006	0.016	0.004	0.041
NWY	86	12	561	561	559 |	0.022	0.006	-0.004	0.008	0.006	0.014	0.004	0.043
SLNO	85	17	651	651	648 |	0.028	0.007	-0.003	0.004	0.006	0.012	0.005	0.042
BNY	86	16	717	717	715 |	0.024	0.008	-0.004	0.008	0.007	0.016	0.004	0.036
NHCT	86	15	578	578	573 |	0.027	0.011	-0.002	0.001	0.006	0.016	0.004	0.038
MTN	84	7	1353	1353	1351 |	0.041	0.008	-0.002	-0.006	0.006	0.013	0.005	0.036
C1IL	86	10	1233	1233	1229 |	0.025	0.008	-0.004	0.010	0.007	0.014	0.004	0.034
ALL		491	757	757	756 |	0.034	0.008	-0.002	-0.004	0.006	0.014	0.005	0.041

Table 4. (cont.)

CLUSTER 3,6 CAL_MISSING

City	Yr	Sam#	NMHC	CBTOT	CLTOT		MPRPE	MTBUT	MALK4	MALK7	MTOL	MXYL	MTMB	MNR
BMTX	86	12	688	687	687	|	0.036	0.007	-0.008	-0.014	0.003	0.007	0.001	0.051
LCLA	85	15	740	740	739	|	0.025	0.006	-0.007	-0.012	0.003	0.008	0.003	0.079
TCTX	84	12	808	808	808	|	0.043	0.007	-0.008	-0.007	0.003	0.007	0.004	0.085
BRLA	85	14	547	547	546	|	0.029	0.006	-0.006	-0.007	0.004	0.009	0.003	0.059
H1TX	85	20	806	806	805	|	0.035	0.010	-0.004	-0.008	0.006	0.008	0.002	0.059
ORTX	84	7	583	583	581	|	0.059	0.006	-0.006	-0.007	0.004	0.009	0.005	0.058
ORTX	85	12	616	616	614	|	0.048	0.009	-0.007	-0.015	0.003	0.009	0.003	0.059
H1TX	86	13	1205	1205	1204	|	0.021	0.009	-0.011	-0.018	0.004	0.009	0.002	0.044
TLOK	86	15	470	470	469	|	0.024	0.004	-0.009	-0.015	0.003	0.008	0.002	0.049
BMTX	84	9	1013	1013	1012	|	0.030	0.006	-0.015	-0.024	0.003	0.006	0.003	0.053
S1UT	86	15	1289	1289	1288	|	0.027	0.007	-0.005	-0.006	0.004	0.007	0.002	0.034
BMTX	85	14	1360	1360	1356	|	0.092	0.066	-0.007	0.010	0.007	0.012	0.004	0.033
ALL		158	851	851	850	|	0.040	0.016	-0.008	-0.009	0.004	0.008	0.003	0.052

CLUSTER 8

City	Yr	Sam#	NMHC	CBTOT	CLTOT		MPRPE	MTBUT	MALK4	MALK7	MTOL	MXYL	MTMB	MNR
PTNE	85	10	624	624	619	|	0.001	0.032	0.030	-0.006	-0.001	0.007	0.013	0.016
D1CO	86	14	866	866	858	|	0.001	0.018	0.030	-0.005	-0.001	0.008	0.013	0.025
PHPA	86	12	429	429	424	|	0.000	0.015	0.023	-0.005	-0.001	0.009	0.015	0.016
TCTX	85	13	549	549	543	|	0.001	0.027	0.032	-0.005	-0.001	0.008	0.013	0.017
KCMO	84	11	973	973	967	|	0.000	0.025	0.026	-0.009	-0.002	0.007	0.018	0.017
ALL		60	690	689	687	|	0.035	0.008	-0.004	-0.012	0.005	0.011	0.003	0.042

NOT INCLUDED IN ANY OTHER CLUSTER

CLTX	85	11	623	623	621	|	0.061	0.006	-0.002	0.009	0.007	0.007	0.003	0.055

Cluster Averages Repeated Here!

	Sam#	NMHC	CBTOT	CLTOT		MPRPE	MTBUT	MALK4	MALK7	MTOL	MXYL	MTMB	MNR
Ave 1	53	635	635	633	|	0.036	0.007	-0.002	0.003	0.007	0.016	0.005	0.040
Ave 2,4,	491	757	757	756	|	0.034	0.008	-0.002	-0.004	0.006	0.014	0.005	0.041
Ave 3,6	158	851	851	850	|	0.040	0.016	-0.008	-0.009	0.004	0.008	0.003	0.052
Ave 8	60	690	689	687	|	0.035	0.008	-0.004	-0.012	0.005	0.011	0.003	0.042

City	Yr	Sam#	NMHC	CBTOT	CLTOT		MPRPE	MTBUT	MALK4	MALK7	MTOL	MXYL	MTMB	MNR
ALL	ALL	773	761	761	759	|	0.036	0.010	-0.003	-0.005	0.006	0.012	0.004	0.043

Table 5. Carbon Fractions for Aloft Hydrocarbon Data.

Last Update: October CB4

City	Yr	CamID	NMHC	PAR	ETH	OLE	ALD	TOL	XYL	HR	UNK	FOR	CBTOT
PHIL	86	07306C	19	0.442	0.021	0.004	0.037	0.042	0.037	0.370	0.005	0.042	21
PHIL	86	07116B	24	0.325	0.008	0.003	0.059	0.035	0.151	0.150	0.195	0.074	27
PHIL	86	07276C	24	0.345	0.012	0.003	0.108	0.065	0.041	0.235	0.029	0.162	28
PHIL	86	07256C	52	0.498	0.096	0.023	0.003	0.116	0.067	0.081	0.107	0.009	58
PHIL	86	07276B	65	0.419	0.108	0.024	0.033	0.098	0.050	0.105	0.102	0.062	73
PHIL	86	ALL	37	0.421	0.070	0.016	0.039	0.085	0.065	0.149	0.096	0.060	41
ATLA	85	08195B	18	0.444	0.022	0.079	0.029	0.047	0.028	0.312	0.000	0.039	20
ATLA	85	08215C	18	0.544	0.027	0.010	0.028	0.053	0.016	0.292	0.000	0.028	21
ATLA	85	08195A	19	0.446	0.021	0.065	0.028	0.077	0.026	0.279	0.021	0.037	22
ATLA	85	08195C	24	0.428	0.013	0.059	0.022	0.054	0.042	0.239	0.116	0.026	27
ATLA	85	08235A	24	0.428	0.025	0.013	0.029	0.049	0.025	0.326	0.073	0.033	28
ATLA	85	08215B	27	0.392	0.023	0.029	0.020	0.056	0.050	0.227	0.067	0.137	30
ATLA	85	08225C	31	0.486	0.032	0.009	0.017	0.040	0.016	0.377	0.000	0.023	35
ATLA	85	08205C	64	0.728	0.008	0.050	0.008	0.053	0.008	0.118	0.018	0.010	73
ATLA	85	ALL	28	0.530	0.019	0.039	0.020	0.053	0.023	0.245	0.035	0.037	32
DALL	85	07125A	19	0.501	0.027	0.009	0.009	0.056	0.043	0.303	0.000	0.052	21
DALL	85	07125C	19	0.437	0.027	0.020	0.019	0.034	0.024	0.344	0.035	0.061	21
DALL	85	07135A	20	0.423	0.026	0.009	0.018	0.023	0.049	0.307	0.073	0.073	22
DALL	85	07115A	25	0.489	0.016	0.015	0.014	0.036	0.033	0.174	0.088	0.134	28
DALL	85	07135C	27	0.443	0.026	0.003	0.013	0.029	0.011	0.280	0.123	0.072	31
DALL	85	07085B	47	0.412	0.023	0.005	0.034	0.032	0.028	0.327	0.046	0.095	54
DALL	85	ALL	26	0.444	0.024	0.009	0.020	0.034	0.030	0.292	0.062	0.085	29
BIRM	85	08285A	16	0.563	0.012	0.011	0.033	0.115	0.043	0.168	0.016	0.038	18
BIRM	85	08265A	23	0.445	0.031	0.012	0.038	0.034	0.026	0.300	0.071	0.042	26
BIRM	85	08265B	28	0.491	0.039	0.013	0.019	0.023	0.018	0.376	0.000	0.022	32
BIRM	85	ALL	22	0.493	0.030	0.012	0.029	0.049	0.027	0.300	0.028	0.033	26
NEW	86	08056B	19	0.396	0.011	0.004	0.074	0.039	0.005	0.335	0.049	0.088	22
NEW	86	08096C	19	0.406	0.003	0.004	0.098	0.050	0.082	0.318	0.000	0.040	22
NEW	86	07216C	21	0.369	0.048	0.011	0.008	0.086	0.069	0.254	0.138	0.017	24
NEW	86	08116A	23	0.455	0.017	0.004	0.052	0.031	0.017	0.365	0.000	0.059	27
NEW	86	08146A	23	0.445	0.038	0.003	0.074	0.084	0.059	0.207	0.015	0.074	27
NEW	86	08116B	26	0.436	0.002	0.003	0.007	0.031	0.043	0.360	0.089	0.031	29
NEW	86	08116C	31	0.404	0.007	0.003	0.052	0.024	0.003	0.329	0.072	0.106	35
NEW	86	07236C	61	0.509	0.055	0.018	0.032	0.116	0.027	0.087	0.115	0.042	69
NEW	86	ALL	28	0.442	0.027	0.008	0.046	0.066	0.035	0.251	0.070	0.056	32

Table 5. (cont.)

			CB4								
City Yr CanID	NMHC	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR	CBTOT
TULS 85 07205A	18	0.388	0.028	0.013	0.010	0.031	0.022	0.382	0.000	0.127	20
TULS 85 07205C	22	0.307	0.022	0.003	0.132	0.026	0.004	0.241	0.117	0.148	26
TULS 85 07215C	25	0.492	0.033	0.005	0.007	0.023	0.020	0.334	0.021	0.064	28
TULS 85 07165C	26	0.415	0.019	0.126	0.007	0.009	0.012	0.183	0.141	0.089	29
TULS 85 07225A	26	0.502	0.038	0.009	0.053	0.022	0.015	0.345	0.000	0.016	30
TULS 85 07175A	27	0.448	0.027	0.014	0.007	0.039	0.027	0.261	0.092	0.087	30
TULS 85 07165B	28	0.381	0.030	0.002	0.148	0.012	0.003	0.271	0.104	0.047	34
TULS 85 07245C	28	0.490	0.036	0.010	0.013	0.014	0.007	0.290	0.055	0.085	32
TULS 85 07165A	29	0.409	0.021	0.064	0.012	0.017	0.046	0.212	0.115	0.103	32
TULS 85 07235B	29	0.458	0.041	0.004	0.065	0.015	0.010	0.366	0.000	0.042	34
TULS 85 07245B	30	0.424	0.029	0.026	0.080	0.013	0.008	0.228	0.049	0.143	35
TULS 85 07185A	34	0.534	0.032	0.039	0.005	0.020	0.021	0.290	0.021	0.039	39
TULS 85 07215B	36	0.472	0.027	0.023	0.086	0.019	0.014	0.283	0.054	0.022	42
TULS 85 07225B	41	0.424	0.032	0.004	0.060	0.021	0.002	0.274	0.146	0.036	47
TULS 85 07185B	42	0.491	0.032	0.009	0.004	0.022	0.007	0.315	0.033	0.088	47
TULS 85 07225B	50	0.347	0.043	0.006	0.118	0.021	0.008	0.235	0.141	0.080	58
TULS 85 07235A	53	0.454	0.040	0.005	0.030	0.011	0.008	0.356	0.010	0.087	61
TULS 85 07185C	60	0.448	0.019	0.015	0.027	0.040	0.039	0.182	0.134	0.098	68
TULS 85 07235C	65	0.409	0.035	0.010	0.008	0.017	0.014	0.306	0.109	0.092	73
TULS 85 07195C	80	0.506	0.021	0.030	0.044	0.032	0.015	0.216	0.044	0.092	91
TULS 85 07235C	85	0.517	0.050	0.003	0.006	0.007	0.004	0.345	0.000	0.069	97
TULS 85 07195B	86	0.532	0.026	0.020	0.023	0.034	0.021	0.230	0.029	0.085	97
TULS 85 07205B	88	0.587	0.027	0.029	0.016	0.019	0.000	0.249	0.047	0.026	100
TULS 85 ALL	44	0.470	0.031	0.019	0.037	0.021	0.013	0.273	0.061	0.074	50

City Yr CanID	NMHC	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR	CBTOT
ALL TRUE AVE	35	0.468	0.032	0.019	0.035	0.039	0.024	0.257	0.061	0.066	40
MAX	88	0.728	0.108	0.126	0.148	0.116	0.151	0.382	0.195	0.162	100
MIN	16	0.307	0.002	0.002	0.003	0.007	0.000	0.081	0.000	0.009	18

Table 5. (cont.)

			CAL															
City	Yr	CanID	NMHC	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK	CLTOT	Samp
PHIL	86	07306C	19	0.324	0.124	0.021	0.004	0.002	0.042	0.037	0.000	0.042	0.037	0.000	0.167	0.195	0.005	21	
PHIL	86	07116B	24	0.215	0.119	0.008	0.003	0.002	0.035	0.144	0.000	0.074	0.059	0.000	0.071	0.075	0.195	27	
PHIL	86	07276C	24	0.246	0.096	0.012	0.003	0.002	0.065	0.039	0.000	0.162	0.108	0.000	0.117	0.121	0.029	28	
PHIL	86	07256C	52	0.246	0.253	0.096	0.006	0.019	0.116	0.063	0.000	0.009	0.003	0.000	0.042	0.040	0.107	58	
PHIL	86	07276B	65	0.235	0.196	0.108	0.005	0.021	0.098	0.047	0.000	0.062	0.033	0.000	0.042	0.051	0.102	73	
PHIL	86	ALL	37	0.246	0.181	0.070	0.005	0.013	0.085	0.062	0.000	0.060	0.039	0.000	0.069	0.075	0.096	41	5
ATLA	85	08195B	18	0.295	0.123	0.022	0.012	0.071	0.047	0.027	0.000	0.039	0.029	0.000	0.165	0.169	0.000	20	
ATLA	85	08215C	18	0.368	0.206	0.027	0.004	0.009	0.053	0.016	0.000	0.028	0.028	0.000	0.112	0.148	0.000	21	
ATLA	85	08195A	19	0.293	0.136	0.021	0.022	0.051	0.077	0.025	0.000	0.037	0.028	0.000	0.140	0.149	0.021	22	
ATLA	85	08195C	24	0.246	0.168	0.013	0.009	0.054	0.054	0.039	0.000	0.026	0.022	0.000	0.121	0.131	0.116	27	
ATLA	85	08235A	24	0.318	0.105	0.025	0.017	0.002	0.049	0.023	0.000	0.033	0.029	0.000	0.154	0.173	0.073	28	
ATLA	85	08215B	27	0.272	0.129	0.023	0.016	0.018	0.056	0.046	0.000	0.137	0.020	0.000	0.102	0.113	0.067	30	
ATLA	85	08225C	31	0.342	0.149	0.032	0.010	0.003	0.040	0.015	0.000	0.023	0.017	0.000	0.165	0.205	0.000	35	
ATLA	85	08205C	64	0.572	0.189	0.008	0.010	0.044	0.053	0.007	0.000	0.010	0.008	0.000	0.020	0.061	0.018	73	
ATLA	85	ALL	28	0.381	0.157	0.019	0.012	0.031	0.053	0.022	0.000	0.037	0.020	0.000	0.104	0.130	0.035	32	8
DALL	85	07125A	19	0.412	0.112	0.027	0.012	0.002	0.056	0.039	0.000	0.052	0.009	0.000	0.123	0.156	0.000	21	
DALL	85	07125C	19	0.311	0.124	0.027	0.028	0.002	0.034	0.022	0.000	0.061	0.019	0.000	0.156	0.182	0.035	21	
DALL	85	07135A	20	0.291	0.138	0.026	0.011	0.002	0.023	0.044	0.000	0.073	0.018	0.000	0.141	0.161	0.073	22	
DALL	85	07115A	25	0.376	0.143	0.016	0.021	0.002	0.036	0.030	0.000	0.134	0.014	0.000	0.050	0.089	0.088	28	
DALL	85	07135C	27	0.349	0.119	0.026	0.005	0.001	0.029	0.011	0.000	0.072	0.013	0.000	0.115	0.136	0.123	31	
DALL	85	07085B	47	0.276	0.134	0.023	0.003	0.003	0.032	0.025	0.000	0.095	0.034	0.000	0.155	0.175	0.046	54	
DALL	85	ALL	26	0.327	0.129	0.024	0.011	0.002	0.034	0.027	0.000	0.085	0.020	0.000	0.126	0.151	0.062	29	6
BIRM	85	08285A	16	0.367	0.214	0.012	0.014	0.002	0.115	0.042	0.000	0.038	0.033	0.000	0.060	0.085	0.016	18	
BIRM	85	08265A	23	0.374	0.094	0.031	0.003	0.010	0.034	0.024	0.000	0.042	0.038	0.000	0.122	0.156	0.071	26	
BIRM	85	08265B	28	0.421	0.093	0.039	0.008	0.009	0.023	0.017	0.000	0.022	0.019	0.000	0.156	0.195	0.000	32	
BIRM	85	ALL	22	0.392	0.122	0.030	0.008	0.008	0.049	0.025	0.000	0.033	0.029	0.000	0.121	0.155	0.028	26	3
NEW	86	08056B	19	0.280	0.112	0.011	0.004	0.002	0.039	0.005	0.000	0.088	0.074	0.000	0.160	0.177	0.049	22	
NEW	86	08096C	19	0.309	0.096	0.003	0.004	0.002	0.050	0.078	0.000	0.040	0.098	0.000	0.153	0.168	0.000	22	
NEW	86	07216C	21	0.258	0.102	0.048	0.015	0.002	0.086	0.062	0.000	0.017	0.008	0.000	0.130	0.134	0.138	24	
NEW	86	08116A	23	0.362	0.105	0.017	0.005	0.002	0.031	0.015	0.000	0.059	0.052	0.000	0.159	0.193	0.000	27	
NEW	86	08146A	23	0.287	0.164	0.038	0.003	0.002	0.084	0.055	0.000	0.074	0.074	0.000	0.093	0.110	0.015	27	
NEW	86	08116B	26	0.339	0.107	0.002	0.003	0.002	0.031	0.039	0.000	0.031	0.007	0.000	0.160	0.192	0.089	29	
NEW	86	08116C	31	0.307	0.100	0.007	0.004	0.001	0.024	0.003	0.000	0.106	0.052	0.000	0.146	0.178	0.072	35	
NEW	86	07236C	61	0.232	0.263	0.055	0.001	0.017	0.116	0.026	0.000	0.042	0.032	0.000	0.055	0.046	0.115	69	
NEW	86	ALL	28	0.287	0.153	0.027	0.004	0.006	0.066	0.032	0.000	0.056	0.046	0.000	0.119	0.133	0.070	32	8

Table 5. (cont.)

			CAL														
City	Yr	CanID	NMHC	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK	CLTOT
TULS	85	07205A	18	0.247	0.106	0.028	0.007	0.009	0.031	0.021	0.000	0.127	0.010	0.000	0.198	0.217	0.000	20
TULS	85	07205C	22	0.230	0.079	0.022	0.003	0.002	0.026	0.004	0.000	0.148	0.132	0.000	0.111	0.127	0.117	26
TULS	85	07215C	25	0.357	0.147	0.033	0.003	0.003	0.023	0.019	0.000	0.064	0.007	0.000	0.144	0.178	0.021	28
TULS	85	07165C	26	0.285	0.099	0.019	0.003	0.124	0.009	0.011	0.000	0.089	0.007	0.000	0.114	0.099	0.141	29
TULS	85	07225A	26	0.385	0.134	0.038	0.012	0.002	0.022	0.014	0.000	0.016	0.053	0.000	0.139	0.185	0.000	30
TULS	85	07175A	27	0.286	0.163	0.027	0.012	0.006	0.039	0.025	0.000	0.087	0.007	0.000	0.122	0.135	0.092	30
TULS	85	07165B	28	0.288	0.106	0.030	0.002	0.001	0.012	0.003	0.000	0.047	0.148	0.000	0.111	0.146	0.104	34
TULS	85	07245C	28	0.394	0.126	0.036	0.003	0.009	0.014	0.007	0.000	0.085	0.013	0.000	0.108	0.151	0.055	32
TULS	85	07165A	29	0.280	0.119	0.021	0.003	0.062	0.017	0.041	0.000	0.103	0.012	0.000	0.114	0.112	0.115	32
TULS	85	07235B	29	0.372	0.100	0.041	0.003	0.003	0.015	0.010	0.000	0.042	0.065	0.000	0.156	0.194	0.000	34
TULS	85	07245B	30	0.336	0.114	0.029	0.018	0.016	0.013	0.007	0.000	0.143	0.080	0.000	0.080	0.116	0.049	35
TULS	85	07185A	34	0.386	0.174	0.032	0.009	0.033	0.020	0.020	0.000	0.039	0.005	0.000	0.110	0.150	0.021	39
TULS	85	07215B	36	0.348	0.135	0.027	0.007	0.020	0.019	0.013	0.000	0.022	0.086	0.000	0.121	0.150	0.054	42
TULS	85	07225B	41	0.335	0.086	0.032	0.013	0.002	0.021	0.002	0.000	0.036	0.060	0.000	0.121	0.145	0.146	47
TULS	85	07185B	42	0.361	0.150	0.032	0.008	0.004	0.022	0.007	0.000	0.088	0.004	0.000	0.127	0.164	0.033	47
TULS	85	07225B	50	0.315	0.054	0.043	0.004	0.005	0.021	0.007	0.000	0.080	0.118	0.000	0.090	0.121	0.141	58
TULS	85	07235A	53	0.371	0.104	0.040	0.007	0.002	0.011	0.007	0.000	0.087	0.030	0.000	0.143	0.189	0.010	61
TULS	85	07185C	60	0.286	0.183	0.019	0.013	0.007	0.040	0.035	0.000	0.098	0.027	0.000	0.069	0.091	0.134	68
TULS	85	07235C	65	0.328	0.104	0.035	0.012	0.003	0.017	0.013	0.000	0.092	0.008	0.000	0.121	0.159	0.109	73
TULS	85	07195C	80	0.367	0.164	0.021	0.012	0.022	0.032	0.014	0.000	0.092	0.044	0.000	0.083	0.104	0.044	91
TULS	85	07235C	85	0.442	0.129	0.050	0.004	0.000	0.007	0.003	0.000	0.069	0.006	0.000	0.113	0.177	0.000	97
TULS	85	07195B	86	0.366	0.213	0.026	0.011	0.013	0.034	0.020	0.000	0.085	0.023	0.000	0.067	0.113	0.029	97
TULS	85	07205B	88	0.509	0.112	0.027	0.025	0.013	0.019	0.000	0.000	0.026	0.016	0.000	0.074	0.131	0.047	100
TULS	85	ALL	44	0.360	0.132	0.031	0.010	0.013	0.021	0.012	0.000	0.074	0.037	0.000	0.106	0.142	0.061	50

City	Yr	CanID	NMHC	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK	CLTOT
ALL	TRUE	AVE	35	0.341	0.142	0.032	0.009	0.013	0.039	0.023	0.000	0.066	0.035	0.000	0.106	0.134	0.061	40
MAX			88	0.572	0.263	0.108	0.028	0.124	0.116	0.144	0.000	0.162	0.148	0.000	0.198	0.217	0.195	
MIN			16	0.215	0.054	0.002	0.001	0.000	0.007	0.000	0.000	0.009	0.003	0.000	0.020	0.040	0.000	

Table 6. Carbon Fractions for UNC Autoexhaust Analyses.

CB4

Vehicle	Conditions	PAR	ETH	OLE	ALD	TOL	XYL	NR	UNK	FOR	CBTOT
Charger	Fed. Test	0.382	0.107	0.044	0.014	0.139	0.155	0.125	0.026	0.008	1.000
Charger	Hi Idle	0.439	0.062	0.033	0.024	0.154	0.157	0.066	0.058	0.008	1.000
Volare	Fed. Test	0.415	0.121	0.039	0.013	0.103	0.135	0.128	0.039	0.007	1.000
Volare	Hi Idle	0.574	0.044	0.018	0.026	0.104	0.102	0.075	0.050	0.007	1.000
ALL	ALL	0.452	0.084	0.033	0.019	0.125	0.137	0.098	0.043	0.008	1.000

CAL

Vehicle	Conditions	ALK4	ALK7	ETH	PRPE	TBUT	TOL	XYL	TMB	FORM	ALD	RCHO	MISS	NR	UNK
Charger	Fed. Test	0.086	0.196	0.107	0.058	0.027	0.133	0.115	0.046	0.000	0.000	0.000	0.125	0.079	0.025
Charger	Hi Idle	0.113	0.269	0.064	0.044	0.034	0.149	0.117	0.046	0.000	0.000	0.000	0.072	0.034	0.058
Volare	Fed. Test	0.096	0.202	0.122	0.052	0.024	0.098	0.102	0.040	0.000	0.000	0.000	0.136	0.089	0.039
Volare	Hi Idle	0.151	0.335	0.048	0.024	0.034	0.100	0.082	0.025	0.000	0.000	0.000	0.096	0.057	0.050
ALL	ALL	0.111	0.251	0.085	0.044	0.030	0.120	0.104	0.039	0.000	0.000	0.000	0.107	0.065	0.043

Charger= Dodge, Charger
Volare= Plymouth, Volare

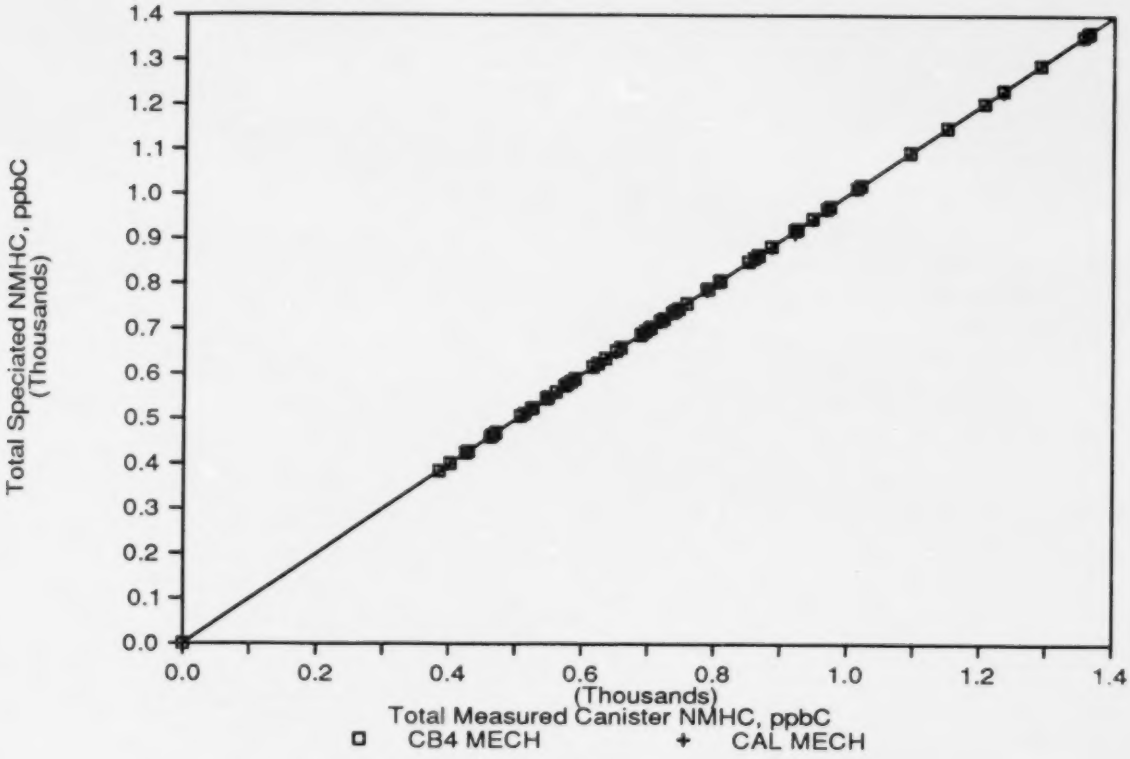

Figure 10. CB4 and CAL sum of species plotted against canister NMOC.

Carbon Class Fractions

Figure 11 shows the carbon fraction in CB4 that is represented by TOL verses the carbon fraction in CAL that is represented by TOL. Although both mechanisms use the explicit chemistry of toluene to represent all mono-alkylated aromatics, and for the most part, both models do treat most mono-alkylated species the same way, there are differences as can be seen in Figure 11. CB4 tends to classify more carbon as TOL than does CAL. In the CB4 mechanism, XYL is used for all aromatics higher than toluene, while in the CAL mechanism, two surrogates are used, XYL (with explicit xylene chemistry) and TMB (with explicit tri-methyl-benzene chemistry). Figure 12 shows the sum of the CAL XYL and TMB fractions verses the CB4 XYL fraction. As shown by this figure, and unlike the TOL species case, the two mechanisms tend to have the same carbon fraction for the higher aromatics.

Figure 13 shows the CAL NR verses the CB4 NR fraction. CAL has on the average one-half the NR as CB4. Figure 14 shows the sum of the CAL ALK4 and ALK7 classes verses the CB4 PAR class. This relationship is scattered, has a slope greater than 1.0 and has a negative intercept. When the CAL sum for

$$\mathrm{ALK4} + \mathrm{ALK7} + \mathrm{MISS} + \mathrm{NR} + (\mathrm{PREP}/3)$$

is plotted verses the CB4 sum for PAR+NR, however, a mostly linear relationship with a slope of about 1.0 results. Therefore, the disagreement for the paraffin class was caused by CAL having a 4-carbon and a 7-carbon molecule to represent all paraffins while CB4 had a 1-carbon entity. For CAL, the difference between the canister average paraffin carbon number and the model's 7-carbon ALK7 is taken up in MISS and NR, but in CB4 this carbon appears directly in PAR.

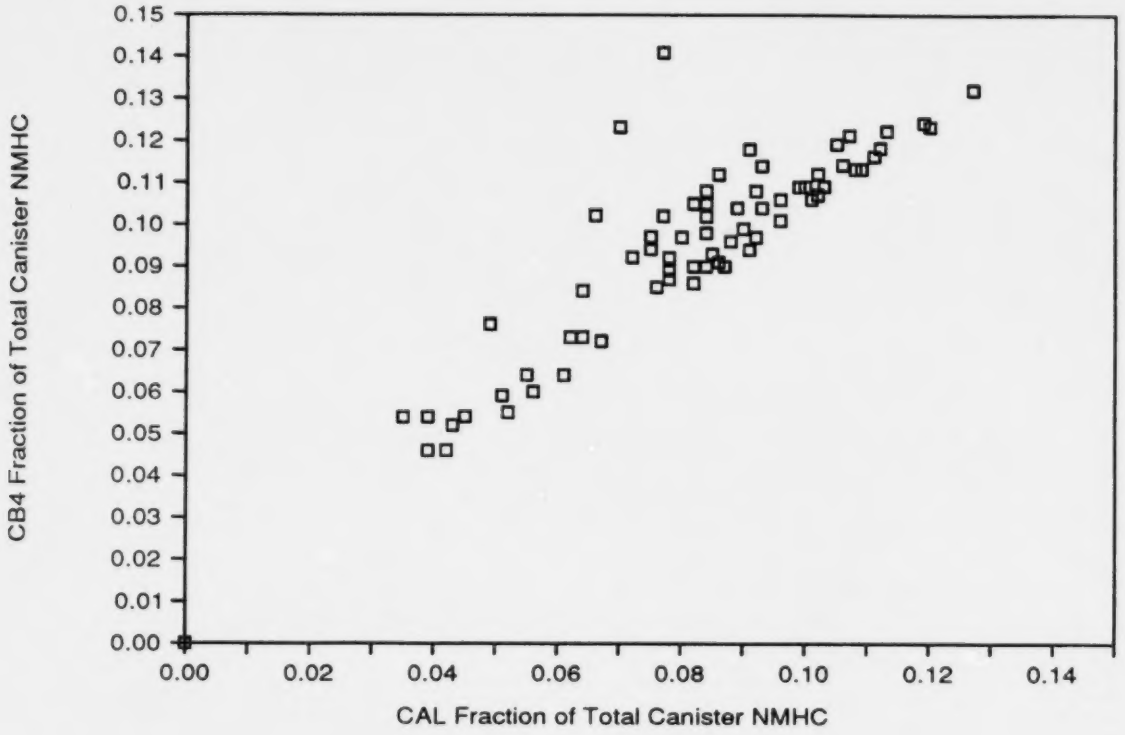

Figure 11. Carbon fraction in CB4 that is represented by TOL vs. carbon fraction in CAL that is represented by TOL.

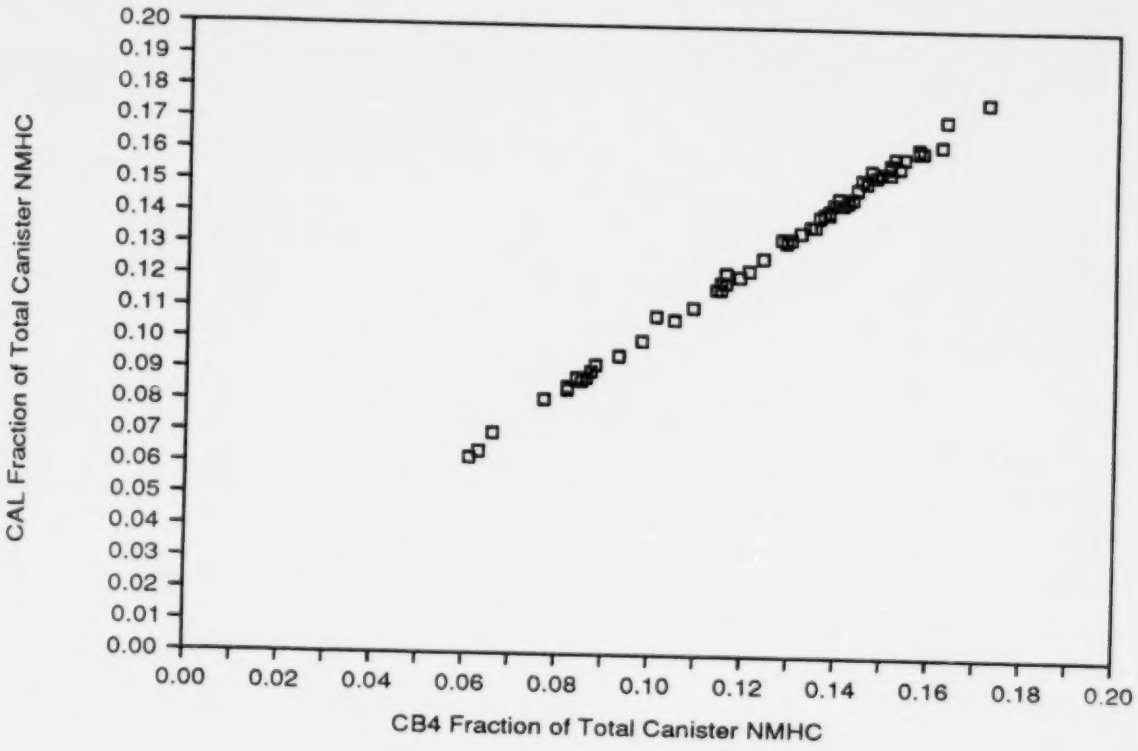

Figure 12. Carbon fraction in CB4 that is represented by XYL vs. carbon fraction in CAL that is represented by XYL+TMB.

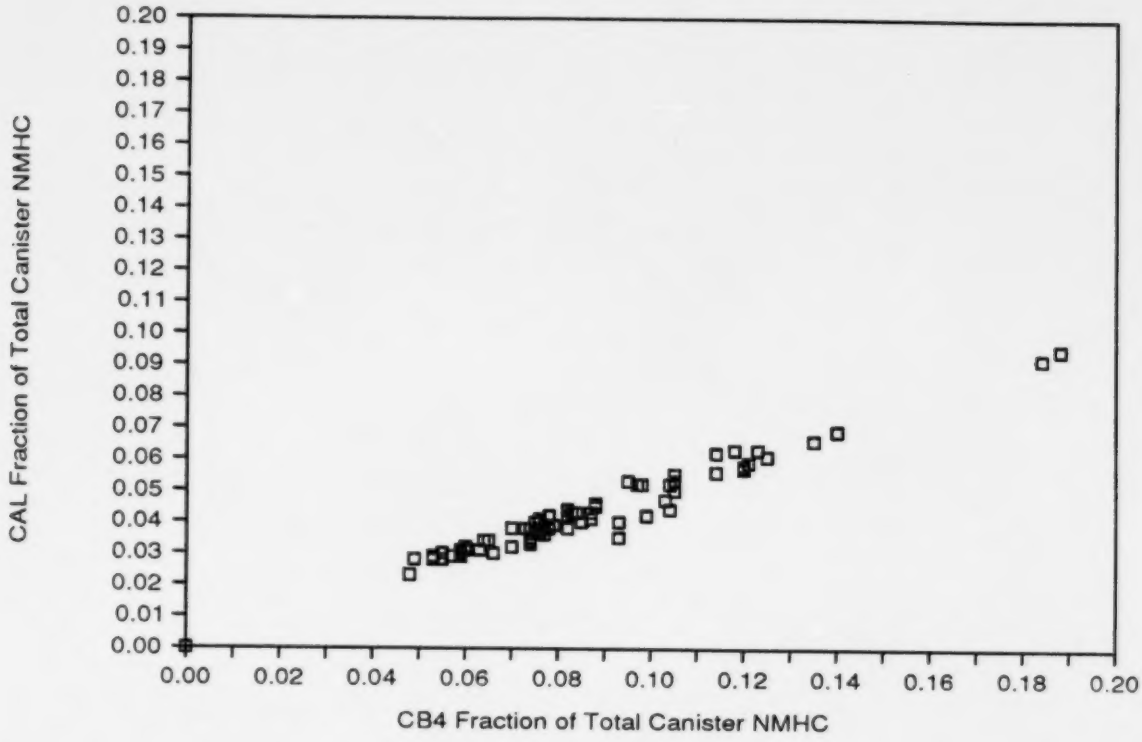

Figure 13. Carbon fraction in CB4 that is represented as NR vs. carbon fraction in CAL that is represented as NR.

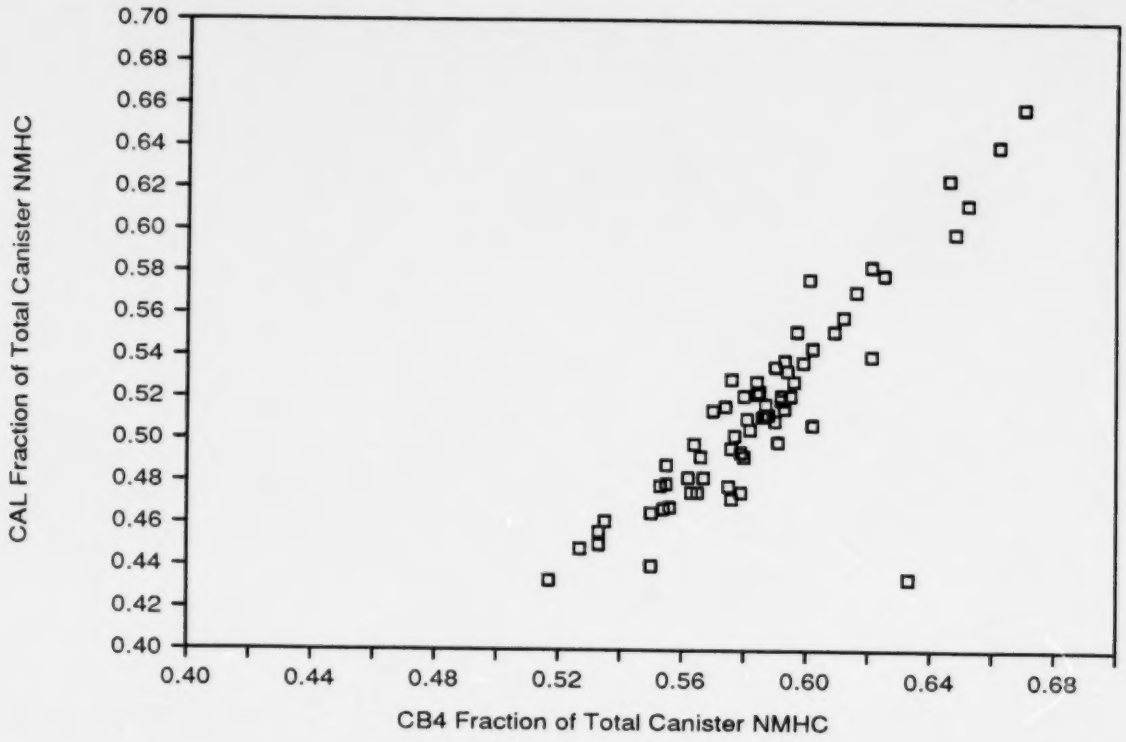

Figure 14. Carbon fraction in CB4's PAR class vs. the sum of the CAL's ALK4 and ALK7 classes.

Cluster Analysis

Cluster analyses are techniques to find samples that are similar in a set of features. Where the features are measured numerically, the Euclidean distance between samples can be used to find groups of samples that are close together in comparison with the distance between the centers of the various groups. For the CB4 carbon fractions, we have points for each city-year in a 9-dimension space, but it will be quite hard to show graphically that collections of certain city-years are "close together" because there are so many dimensions.

There are two basic cluster analysis techniques: joining and k-means algorithms. The joining algorithms assume that there is a rule for computing a distance between any pair of objects and there is a rule for amalgamating any two objects to form a third object. The algorithms proceed by finding the closest pair of objects, removing them from the set of objects, and replacing them by a single amalgamated object. Initially there are as many clusters as there are objects and in the end there is only one. The most common way to illustrate this process is by producing a "tree" with the length of the branches at each level being proportional to the distance between the joined objects at that level. The k-means algorithms also use distances, but begin with a prespecified number of clusters, say n. The goal of the algorithm is to separate the objects into the n clusters so that the means of the clusters are as far a part as possible. That is, the cluster memberships are adjusted until the between-cluster variation is larger than the within-cluster variation. Both cluster methods were used to examine the data in Table 3.

Figure 15 shows one tree produced by a joining method. Reading the tree requires a little study: the vertical lines "join" clusters, the distance from left to right of the joining line suggesting how far apart were the clusters that were joined. This distance is the Euclidean distance between the nearest neighbors of the two clusters. CLTX85 (Clute, Texas, 1985) is far away from all other city-years. On the other hand, there is a large cluster in the middle beginning with RLNC85 (Raleigh NC) and ending with RVA_84 (Ronoke, VA) and including 34 of the 66 city-years that are all very close to each other. Another cluster is evident at the top and yet another at the bottom of the tree. The top cluster has a predominance of Texas and mid-western cities, while the cluster at the bottom has many Eastern cities (*e.g.*, WDC_85, Washington, DC).

Table 7 shows the output from a k-means method with 8 clusters. The number of clusters was varied from 2 to 8 and each output was examined. The k-means algorithm includes an analysis of variance table for the "features" that are used to compute the distance; this table is at the top of Table 7. From the F-ratios which

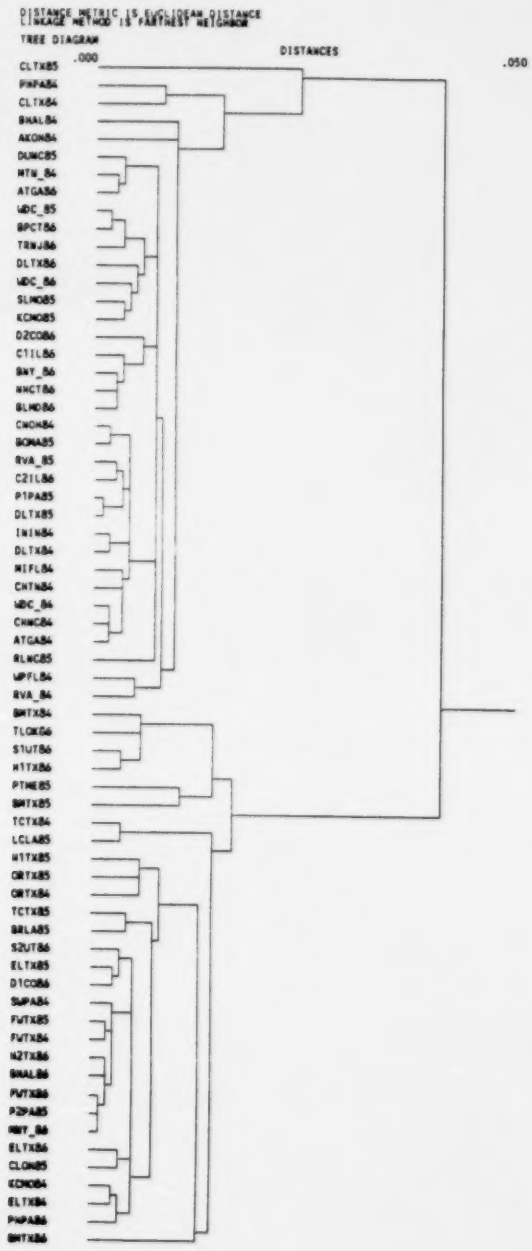

Figure 15. Joining Tree Produced by Cluster Analysis.

estimate the probabilities that the between variances arise merely from chance, given the within variances, we see that the ALD, FORM, and UNK fractions are not very different among the clusters. The strongest differences arise from the PAR, XYL, TOL, and NR fractions. Again we see that CLTX85 (Clute, Texas, 1985) forms its own cluster, that there is a well separated cluster containing WDC_85, and there are two well separated clusters that have "oil and gas" operations-type cities. There is a middle group of clusters (2,4,7) that appear to be quite close (PAR $\approx$ 0.58, XYL $\approx$ 0.15). We decided to form 5 clusters: (1) (2,4,7) (3,6) (8) and, of course, (5) for CLTX85 all by itself. To illustrate graphically the variation among these clusters, the four strongest differences were combined into two dimensions (PAR+NR verses TOL+XYL) and the location of the cluster centers and the cluster members are shown in Figure 16. In looking at this plot, remember that the dimensions have been "flattened" to two-dimensions, and therefore, that two points that may look close together here may, in 9-dimensions, be further apart. Also remember that the sample concentration influences the contribution each point makes to the location of the center of the cluster.

Now the layout of Table 4 should make sense. Furthermore, the identity of the cluster members, each cluster average composition, and the grand average composition are all listed in the table.

Regression Analysis

Yet another way of estimating the grand composition is to do a multiple regression analysis of the data in Table 4. That is, the individual city-year's fractions are converted to actual ppbC carbon for each mechanism species by multiplying by the sample total NMOC. Then we do a regression with the model

$$\text{Total NMOC} = f_1 C_1 + f_2 C_2 \ldots + f_9 C_9$$

where $C_1 \ldots C_9$ are the concentrations of the species which are known and $f_1 \ldots f_9$ are the grand set of coefficients that will result in the sum of the concentrations closely equaling the Total NMOC in a least squares sense. The standardized form of these coefficients will be the best set of least squares estimated carbon fractions for all city-years. Table 8 shows the output of the regression analysis. Figure 17 shows the residuals (difference between the observed and predicted Total NMOC) for each city-year from using the coefficients to calculate the Total NMOC: the errors are between +2 ppbC and -2 ppbC, which is an average error of less than 0.5%. Note, however, that there are a series of nearly uniformly negative residuals and another of nearly uniformly positive residuals. These can be used to select members for at least two clusters (one below the current mean and one above the current mean) and thus reduce the residuals in these clusters even further.

Table 7. Output from a K-means Cluster Method.

SUMMARY STATISTICS FOR 8 CLUSTERS

VARIABLE	BETWEEN SS	DF	WITHIN SS	DF	F-RATIO	PROB
PAR	.066	7	.008	58	65.103	.000
ETH	.017	7	.009	58	16.840	.000
OLE	.002	7	.003	58	5.460	.000
ALD	.000	7	.002	58	2.304	.038
TOL	.024	7	.006	58	31.413	.000
XYL	.053	7	.009	58	50.998	.000
NR	.039	7	.013	58	24.074	.000
FOR	.001	7	.002	58	2.179	.049
UNK	.000	7	.000	58	2.646	.019

CLUSTER NUMBER: 1

MEMBERS		STATISTICS				
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
WDC_85	.01	PAR	.52	.53	.55	.01
BPCT86	.01	ETH	.03	.04	.05	.01
DLTX86	.01	OLE	.03	.03	.04	.00
TRNJ86	.01	ALD	.02	.02	.03	.00
BHAL84	.01	TOL	.08	.10	.12	.02
RVA_84	.02	XYL	.16	.17	.20	.02
		NR	.06	.08	.10	.01
		FOR	.00	.01	.02	.00
		UNK	.00	.00	.01	.00

CLUSTER NUMBER: 2

MEMBERS		STATISTICS				
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
ELTX86	.01	PAR	.55	.58	.60	.01
CLOH85	.01	ETH	.03	.04	.09	.02
P1PA85	.01	OLE	.02	.03	.04	.00
CLTX84	.02	ALD	.01	.02	.04	.01
S2UT86	.01	TOL	.06	.08	.09	.01
ELTX85	.01	XYL	.12	.13	.16	.01
BHAL86	.01	NR	.08	.09	.12	.01
PHPA84	.02	FOR	.00	.01	.03	.01
ELTX84	.01	UNK	.00	.01	.01	.00
FWTX85	.00					
H2TX86	.01					
FWTX84	.00					
AKOH84	.02					
DLTX85	.01					
SWPA84	.01					

Table 7. (cont.)

CLUSTER NUMBER: 3

MEMBERS		STATISTICS				
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
BMTX86	.02	PAR	.58	.60	.62	.01
LCLA85	.02	ETH	.02	.04	.09	.02
TCTX84	.02	OLE	.02	.04	.06	.01
BRLA85	.01	ALD	.01	.02	.02	.00
H1TX85	.01	TOL	.04	.05	.07	.01
ORTX84	.01	XYL	.07	.09	.11	.01
ORTX85	.01	NR	.12	.15	.19	.03
		FOR	.00	.01	.03	.01
		UNK	.00	.01	.02	.00

CLUSTER NUMBER: 4

MEMBERS		STATISTICS				
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
ININ84	.01	PAR	.55	.58	.60	.01
C2IL86	.01	ETH	.00	.03	.04	.01
MIFL84	.01	OLE	.02	.03	.04	.01
BOMA85	.01	ALD	.02	.02	.03	.00
RVA_85	.01	TOL	.07	.09	.11	.01
WDC_84	.00	XYL	.14	.16	.20	.01
DLTX84	.01	NR	.05	.06	.08	.01
CNOH84	.01	FOR	.00	.01	.02	.01
CHNC84	.00	UNK	.00	.01	.01	.00
DUNC85	.01					
ATGA84	.01					
RLNC85	.01					
WPFL84	.02					
CHTN84	.01					

CLUSTER NUMBER: 5

MEMBERS		STATISTICS				
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
CLTX85	.00	PAR	.47	.47	.47	.00
		ETH	.16	.16	.16	.00
		OLE	.07	.07	.07	.00
		ALD	.01	.01	.01	.00
		TOL	.05	.05	.05	.00
		XYL	.09	.09	.09	.00
		NR	.11	.11	.11	.00
		FOR	.03	.03	.03	.00
		UNK	.00	.00	.00	.00

Table 7. (cont.)

CLUSTER NUMBER: 6

MEMBERS			STATISTICS			
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
H1TX86	.01	PAR	.64	.65	.67	.01
TLOK86	.01	ETH	.02	.03	.04	.01
BMTX84	.01	OLE	.02	.04	.07	.02
S1UT86	.01	ALD	.01	.02	.03	.01
BMTX85	.02	TOL	.04	.05	.06	.01
		XYL	.07	.08	.09	.01
		NR	.08	.11	.13	.02
		FOR	.00	.01	.02	.01
		UNK	.00	.00	.00	.00

CLUSTER NUMBER: 7

MEMBERS			STATISTICS			
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
WDC_86	.01	PAR	.55	.57	.58	.01
FWTX86	.01	ETH	.03	.04	.04	.00
P2PA85	.01	OLE	.02	.03	.04	.00
BLMD86	.01	ALD	.02	.02	.04	.01
D2CO86	.01	TOL	.10	.11	.13	.01
KCMO85	.01	XYL	.14	.15	.16	.01
ATGA86	.00	NR	.06	.08	.10	.01
MNY_86	.00	FOR	.00	.01	.01	.00
SLMO85	.01	UNK	.00	.00	.01	.00
BNY_86	.01					
NHCT86	.01					
MTN_84	.01					
C1IL86	.01					

CLUSTER NUMBER: 8

MEMBERS			STATISTICS			
CASE	DISTANCE	VARIABLE	MINIMUM	MEAN	MAXIMUM	ST.DEV.
PTME85	.01	PAR	.61	.62	.65	.02
D1CO86	.01	ETH	.02	.03	.04	.00
PHPA86	.00	OLE	.03	.03	.04	.00
TCTX85	.01	ALD	.02	.02	.04	.01
KCMO84	.01	TOL	.06	.08	.09	.01
		XYL	.10	.12	.13	.01
		NR	.07	.09	.10	.01
		FOR	.00	.01	.01	.00
		UNK	.00	.00	.01	.00

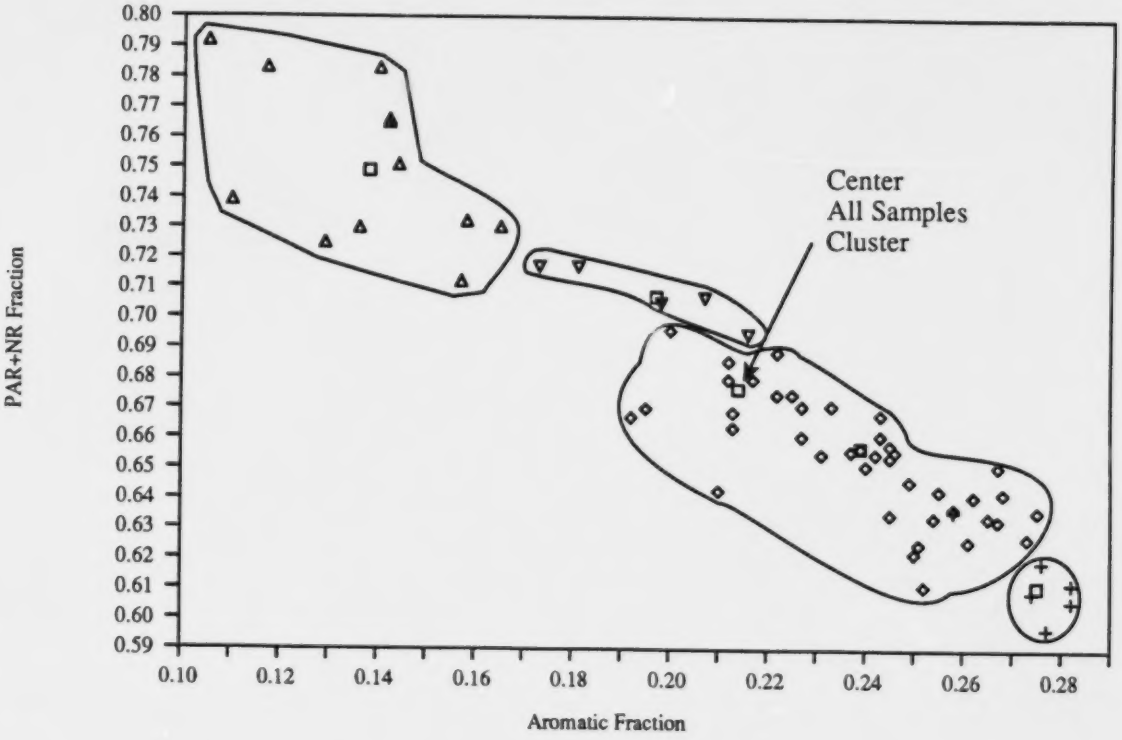

Figure 16. PAR+NR vs. TOL + XYL and the location of the cluster centers and the cluster members.

Table 8. Output of Regression Analysis.

```
MODEL CONTAINS NO CONSTANT.

DEP VAR:    NMHC      N:   66    MULTIPLE R: 1.000    SQUARED MULTIPLE R: 1.000

          2       2
ADJUSTED R = 1-(1-R )*(N-1)/DF, WHERE N=  66, AND DF=  57: 1.000
```

VARIABLE	COEFFICIENT	STD. ERROR	STD. COEF.	TOLERANCE	T	P(2 TAIL)
PAR	1.003	0.002	0.592	0.00850	541.96	.000
ETH	1.003	0.007	0.042	0.12888	150.11	.000
OLE	1.013	0.015	0.037	0.03307	67.56	.000
ALD	0.990	0.027	0.024	0.02458	37.04	.000
TOL	1.000	0.010	0.097	0.01042	98.27	.000
XYL	0.993	0.008	0.126	0.01033	126.88	.000
NR	0.987	0.006	0.088	0.04079	175.65	.000
UNK	1.016	0.018	0.012	0.21891	56.64	.000
FOR	0.856	0.090	0.002	0.37921	9.50	.000

ANALYSIS OF VARIANCE

SOURCE	SUM-OF-SQUARES	DF	MEAN-SQUARE	F-RATIO	P
REGRESSION	.419880E+08	9	4665337.083	10963420.000	.000
RESIDUAL	24.256	57	0.426		

```
INPUT STATEMENTS FOR THIS JOB:

USE ALLCITYC
MODEL NMHC=PAR+ETH+OLE+ALD+TOL+XYL+NR+UNK+FOR
ESTIMATE
```

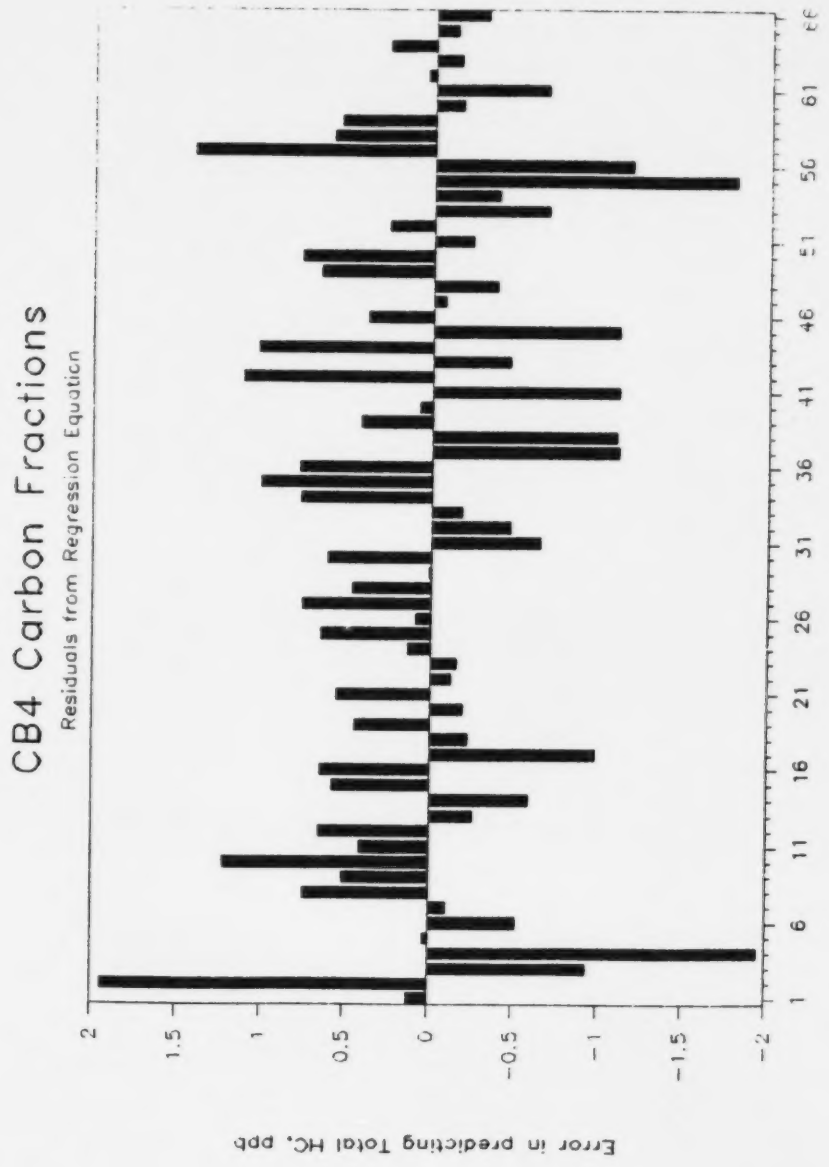

Figure 17. The residuals (difference between the observed and predicted Total NMHC) for each city-year from using the coefficients to calculate the Total NMHC.

Recommended Carbon Fractions

Tables 9a and b summarize the results. The top part of the tables lists the values as they were calculated. The middle part of the tables adjusts the fractions for the UNK fraction, by *assuming that the unknown material had the same species distribution as the rest of the carbon.* Furthermore, because the urban surface method did not include aldehydes in the measurements, 5% additional aldehydes have been added (0.02 HCHO and 0.03 ALD) so that the fractions would total to 1.05. The bottom part of the tables adjust the total to be 1.00 by taking only 95% of the NMOC and adding 5% aldehydes. These latter values for the CB4 mechanism are the default values coded into the OZIPM4 program and will be used automatically to split the user specified NMOC.

Table 9. Recommended Carbon Fractions.

Carbon Bond Four Hydrocarbon Carbon Fractions

Clust	(1)	(2,4,7)	(3,6)	(8)	ALL	Aloft1	Aloft2
Sam#	53	491	158	60	773	53	53
NMHC	635	757	851	690	761	40	40
CBTOT	635	757	851	689	761	40	40
Analysis of City Canisters							
PAR	0.527	0.577	0.627	0.621	0.588	0.464	0.468
ETH	0.043	0.038	0.035	0.031	0.039	0.033	0.032
OLE	0.037	0.033	0.042	0.032	0.036	0.020	0.019
ALD	0.023	0.023	0.023	0.023	0.023	0.035	0.035
TOL	0.121	0.104	0.059	0.089	0.093	0.042	0.039
XYL	0.159	0.137	0.080	0.110	0.122	0.026	0.024
FOR	0.001	0.001	0.001	0.001	0.001	0.066	0.066
NR	0.076	0.077	0.121	0.086	0.088	0.253	0.256
UNK	0.013	0.010	0.012	0.007	0.010	0.061	0.061
Tot	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Recommended Fractions (adj for UNK, 100% HC + 5% aldehydes)							
	(1)	(2,4,7)	(3,6)	(8)	ALL	Aloft1	Aloft2
PAR	0.534	0.583	0.635	0.625	0.594	0.494	0.498
ETH	0.044	0.038	0.035	0.031	0.039	0.035	0.034
OLE	0.037	0.033	0.043	0.032	0.036	0.021	0.020
ALD	0.053	0.053	0.053	0.053	0.053	0.037	0.037
TOL	0.123	0.105	0.060	0.090	0.094	0.045	0.042
XYL	0.161	0.138	0.081	0.111	0.123	0.028	0.026
FOR	0.021	0.021	0.021	0.021	0.021	0.070	0.070
NR	0.077	0.078	0.122	0.087	0.089	0.269	0.273
Tot	1.050	1.050	1.050	1.050	1.050	1.000	1.000
Fractions (adj for UNK, 95% HC + 5% aldehydes)							
	(1)	(2,4,7)	(3,6)	(8)	ALL	Aloft1	Aloft2
PAR	0.507	0.554	0.603	0.594	0.564	0.494	0.498
ETH	0.041	0.036	0.034	0.030	0.037	0.035	0.034
OLE	0.036	0.032	0.040	0.031	0.035	0.021	0.020
ALD	0.052	0.052	0.052	0.052	0.052	0.037	0.037
TOL	0.116	0.100	0.057	0.085	0.089	0.045	0.042
XYL	0.153	0.131	0.077	0.105	0.117	0.028	0.026
FOR	0.021	0.021	0.021	0.021	0.021	0.070	0.070
NR	0.073	0.074	0.116	0.082	0.084	0.269	0.273
Tot	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Table 9. (cont.)

Carter, Atkinson, Lurmann Hydrocarbon Carbon Fractions

Clust	(1)	(2,4,7)	(3,6)	(8)	ALL	Aloft1	Aloft2
Sam#	53	491	158	60	773	53	53
NMHC	635	757	851	690	761	40	40
CLTOT	633	756	850	687	759	40	40
Analysis of City Canisters							
ALK4	0.176	0.198	0.298	0.248	0.223	0.337	0.341
ALK7	0.267	0.304	0.265	0.316	0.292	0.142	0.142
ETH	0.043	0.038	0.035	0.031	0.039	0.033	0.032
PRPE	0.053	0.047	0.057	0.046	0.050	0.009	0.009
TBUT	0.029	0.030	0.032	0.029	0.030	0.014	0.013
TOL	0.107	0.093	0.051	0.078	0.083	0.042	0.039
XYL	0.110	0.091	0.054	0.074	0.082	0.024	0.023
TMB	0.053	0.049	0.029	0.040	0.044	0.000	0.000
FORM	0.000	0.000	0.000	0.000	0.000	0.066	0.066
ALD	0.000	0.000	0.000	0.000	0.000	0.035	0.035
RCHO	0.000	0.000	0.000	0.000	0.000	0.000	0.000
NR	0.038	0.039	0.059	0.043	0.044	0.132	0.134
MISS	0.111	0.101	0.108	0.088	0.103	0.105	0.105
UNK	0.013	0.010	0.012	0.007	0.010	0.061	0.061
Tot	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Recommended Fractions (adj for UNK, 100% HC + 5% aldehydes)

	(1)	(2,4,7)	(3,6)	(8)	ALL	Aloft1	Aloft2
ALK4	0.178	0.200	0.302	0.250	0.225	0.359	0.363
ALK7	0.271	0.307	0.268	0.318	0.295	0.151	0.151
ETH	0.044	0.038	0.035	0.031	0.039	0.035	0.034
PRPE	0.054	0.047	0.058	0.046	0.051	0.010	0.010
TBUT	0.029	0.030	0.032	0.029	0.030	0.015	0.014
TOL	0.108	0.094	0.052	0.079	0.084	0.045	0.042
XYL	0.111	0.092	0.055	0.075	0.083	0.026	0.024
TMB	0.054	0.049	0.029	0.040	0.044	0.000	0.000
FORM	0.020	0.020	0.020	0.020	0.020	0.070	0.070
ALD	0.030	0.030	0.030	0.030	0.030	0.037	0.037
RCHO	0.000	0.000	0.000	0.000	0.000	0.000	0.000
NR	0.151	0.141	0.169	0.132	0.148	0.252	0.255
Tot	1.050	1.050	1.050	1.050	1.050	1.000	1.000

Recommended Fractions (adj for UNK, 95% HC + 5% aldehydes)

	(1)	(2,4,7)	(3,6)	(8)	ALL	Aloft1	Aloft2
ALK4	0.169	0.190	0.287	0.237	0.214	0.359	0.363
ALK7	0.257	0.292	0.255	0.302	0.280	0.151	0.151
ETH	0.041	0.036	0.034	0.030	0.037	0.035	0.034
PRPE	0.051	0.045	0.055	0.044	0.048	0.010	0.010
TBUT	0.028	0.029	0.031	0.028	0.029	0.015	0.014
TOL	0.103	0.089	0.049	0.075	0.080	0.045	0.042
XYL	0.106	0.087	0.052	0.071	0.079	0.026	0.024
TMB	0.051	0.047	0.028	0.038	0.042	0.000	0.000
FORM	0.020	0.020	0.020	0.020	0.020	0.070	0.070
ALD	0.030	0.030	0.030	0.030	0.030	0.037	0.037
RCHO	0.000	0.000	0.000	0.000	0.000	0.000	0.000
NR	0.143	0.134	0.161	0.125	0.141	0.252	0.255
Tot	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Sensitivity to HC Composition

To illustrate the effects of using different HC compositions a series of simple EKMA-like simulations were run. The conditions for these simulations are for a typical test case (the example Philadelphia SIP day) and include the following conditions.

Initial Conditions.

Item	Value	Units
Latitude	39.93	degrees
Longitude	75.10	degrees
Date	6/24/80	mm/dd/yy
Initial Mixing Ht.	250	meter
Final Mixing Ht.	1235	meter
Initial NMOC	1.100	ppmC
Initial NO_x	0.120	ppm
Surface NMOC	0.038	ppmC
Surface O_3	0.010	ppm
Aloft NMOC	0.040	ppmC
Aloft O_3	0.070	ppm
Temperature	303	K
Water Vapor	25000	ppm

Emissions Fractions.

Hour	1	2	3	4	5	6	7	8
NMOC	0.17	0.17	0.17	0.10	0.02	0.02	0.02	0.02
NO_x	0.35	0.35	0.35	0.19	0.03	0.03	0.03	0.07

Figure 18 shows the comparison of CB4 Version 4.2 using the older OAQPS carbon fractions[15] and with the same simulation using the UNC recommended carbon fractions. The new recommended UNC composition is more reactive for the CB4 mechanism.

Figure 19 shows the comparison of CAL with the ERT carbon fractions[2] and with the UNC recommended carbon fractions. The new recommended UNC composition is less reactive for the CAL mechanism.

Figure 20 compares CB4 and CAL predictions using the UNC carbon fractions. Finally, Figure 21 compares CB4 and CAL predictions with three different HC compositions: Cluster 1 (*i.e.*, WDC_85), Cluster 3,6 (*i.e.*, Texas-like), and the average.

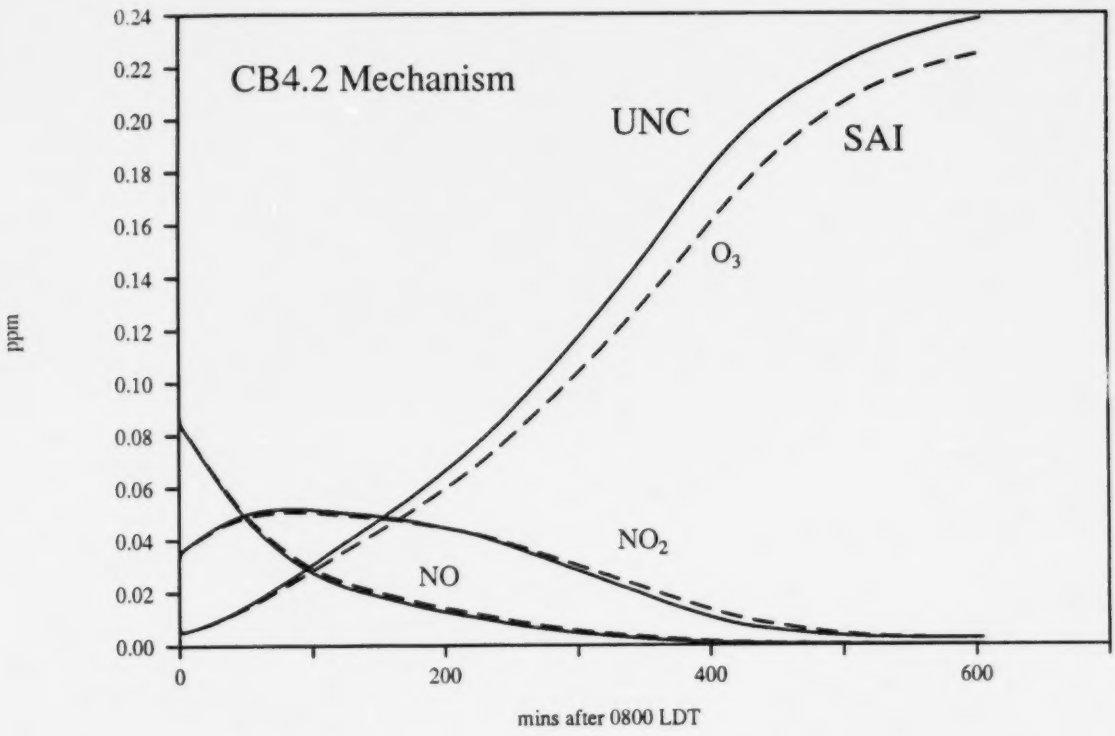

Figure 18. Comparison of CB4 predictions with older SAI fractions to predictions using Table 9 fractions.

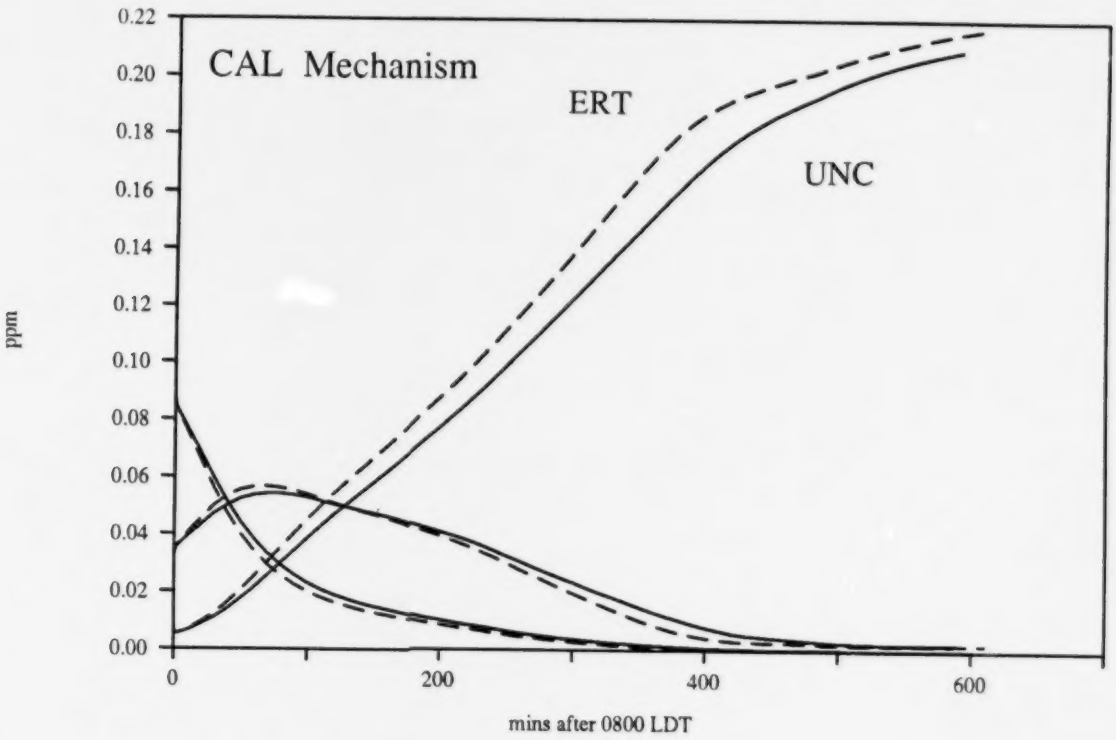

Figure 19. Comparison of CAL predictions with older ERT fractions to predictions using Table 9 fractions.

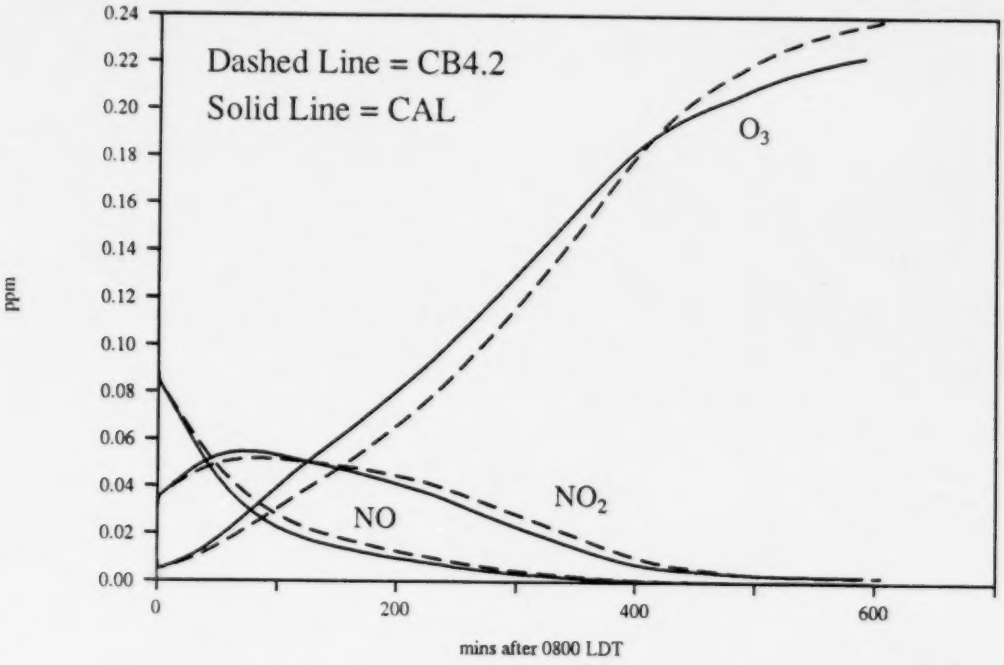

Figure 20. Comparison of CB4 and CAL predictions when both use the UNC Carbon Fractions.

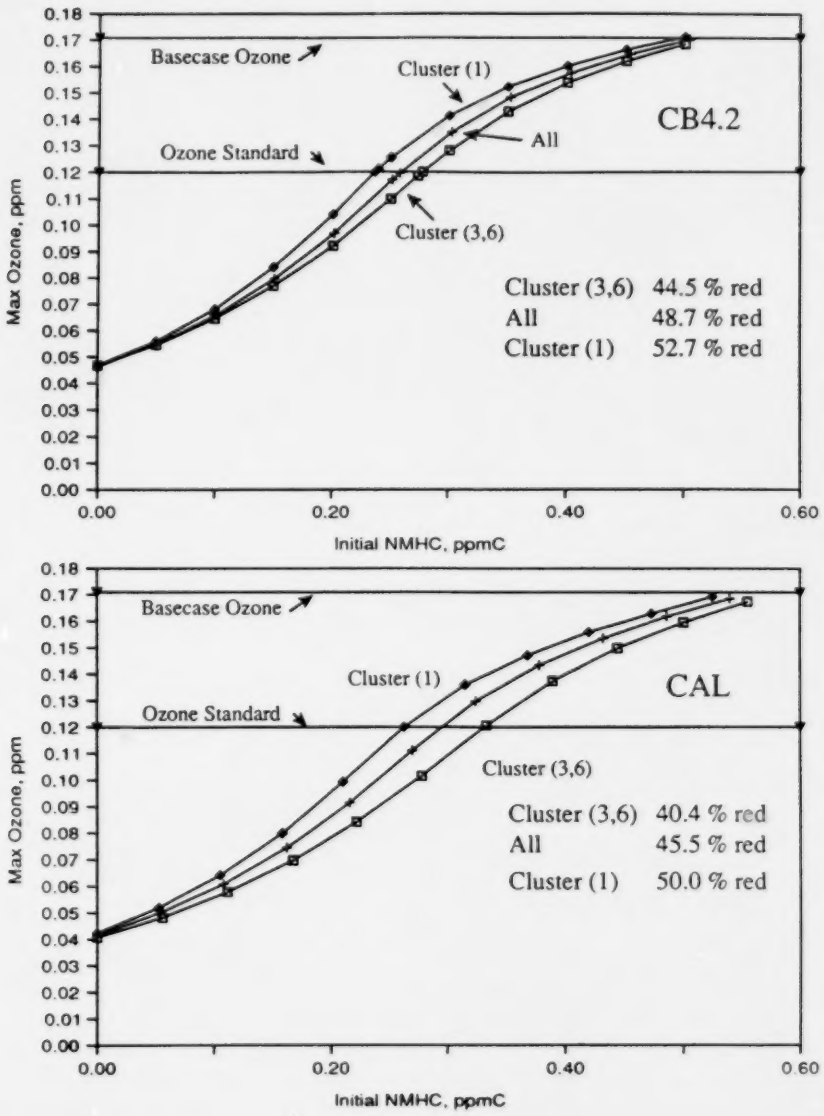

Figure 21. Effect of Hydrocarbon Composition on Ozone Predictions in EKMA simulataion. Cluster 1 is a high traffic condition, *e.g.*, WDC_85 and Cluster 3,6 is Texas-like.

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A

HC Codes and Speciation

Table A.10. EPA assigned HC identification codes, species names, and retention times for ambient HC analysis.

0	unknown	0
101	ETHANE	2.018
102	ETHYLENE	1.83
103	ACETYLENE	1.96
104	PROPENE	2.94
105	PROPANE	3.03
106	Unknown	3.273
107	PARAFFIN	3.46
108	OLEFIN	4.017
109	OLEFIN	4.45
110	ISOBUTANE	5
111	Unknown	5.323
112	Unknown	5.561
113	2-METHYLPROPENE,BUTENE-1	5.995
114	1,3-BUTADIENE	6.166
115	n-BUTANE	6.342
116	t-2-BUTENE	6.817
117	c-2-BUTENE	7.37
118	3-METHYL-1-BUTENE	8.609
119	ISOPENTANE	9.268
120	C5 OLEFIN	9.522
121	1-PENTENE	9.87
122	C5 OLEFIN	9.956
123	2-METHYL-1-BUTENE	10.142
124	n-PENTANE	10.28
125	ISOPRENE	10.43
126	t-2-PENTENE	10.607
127	C5-OLEFIN	10.878
128	2-METHYL-2-BUTENE	10.986
129	c-2-PENTENE	11.042
130	C5 OLEFIN	11.126
131	C6 PARAFFIN	11.375
132	C6 PARAFFIN	11.421
133	2,2-DIMETHYLBUTANE	11.542
134	C6 OLEFIN	11.864
135	C6 OLEFIN	12.122
136	C6 PARAFFIN	12.356
137	4-METHYL-1-PENTENE	12.36
138	CYCLOPENTANE	12.501
139	2,3-DIMETHYLBUTANE	12.633
140	c-4-METHYL-2-PENTENE	12.718
141	2-METHYLPENTANE	12.827
142	t-4-METHYL-2-PENTENE	12.901
143	C6 OLEFIN	12.967
144	C6 OLEFIN	13.239
145	3-METHYLPENTANE	13.31
146	2METHYL1PENTENE,1HEXENE	13.513
147	C6 OLEFIN	13.72
148	n-HEXANE,2-ETHYL-1-BUTENE	13.932
149	C7 PARAFFIN	14.034
150	C7 OLEFIN	14.11
151	2-METHYL-2-PENTENE	14.187
152	C7 OLEFIN	14.276
153	c or t-2-HEXENE	14.413
154	C7 OLEFIN	14.475
155	c&t-3-METHYL-2-PENTENE	14.62

Table A.10, cont

156	METHYLCYCLOPENTANE	14.768
157	2,4-DIMETHYLPENTANE	14.955
158	2,2,3-TRIMETHYL-1-BUTENE	15.047
159	C7 OLEFIN	15.151
160	C7 OLEFIN	15.393
161	C7 PARAFFIN	15.527
162	BENZENE	15.551
163	3,3-DIMETHYLPENTANE	15.748
164	CYCLOHEXANE	15.85
165	C7 OLEFIN	15.926
166	2-METHYLHEXANE	16.19
167	2,3-DIMETHYLPENTANE	16.228
168	CYCLOHEXENE	16.307
169	C7 OLEFIN	16.377
170	3-METHYLHEXANE	16.462
171	C7 PARAFFIN	16.655
172	C7 PARAFFIN	16.786
173	2,2,4-TRIMETHYLPENTANE	16.877
174	C8 OLEFIN	17.186
175	n-HEPTANE	17.228
176	t-HEPTENE-2	17.377
177	C8 OLEFIN	17.537
178	c-HEPTENE-2	17.632
179	METHYLCYCLOHEXANE	17.854
180	25DIMETHYLHEXANE,3MECYCLOHEXEN	18.213
181	2,4-DIMETHYLHEXANE	18.277
182	C8 PARAFFIN	18.472
183	C8 PARAFFIN	18.686
184	2,3,4-TRIMETHYLPENTANE	18.767
185	TOLUENE	18.892
186	C8 PARAFFIN	19.04
187	C8 PARAFFIN	19.072
188	C8 PARAFFIN	19.127
189	2-METHYLHEPTANE	19.231
190	C8 PARAFFIN	19.278
191	3-METHYLHEPTANE	19.455
192	C8 PARAFFIN	19.571
193	2,2,5-TRIMETHYLHEXANE	19.775
194	1-OCTENE	19.871
195	CYCLOHEPTANE	19.979
196	C8 PARAFFIN	20.05
197	C8 PARAFFIN	20.12
198	n-OCTANE	20.2
199	C9 PARAFFIN	20.247
200	C9 PARAFFIN	20.34
201	c-2-OCTENE	20.532
202	C9 PARAFFIN	20.697
203	C9 OLEFIN	20.819
204	2,4-DIMETHYLHEPTANE	20.879
205	C9 PARAFFIN	20.993
206	C9 PARAFFIN	21.042
207	C9 PARAFFIN	21.093
208	ETHYLCYCLOHEXANE	21.147
209	2,5-DIMETHYLHEPTANE	21.239
210	C9 PARAFFIN	21.295
211	C9 PARAFFIN	21.394

Table A.10, cont

212	C9 PARAFFIN	21.466
213	ETHYLBENZENE	21.614
214	2,3-DIMETHYLHEPTANE	21.712
215	m&p-XYLENE	21.843
216	4-METHYLOCTANE	22.01
217	C9 PARAFFIN	22.105
218	3-METHYLOCTANE	22.192
219	C9 PARAFFIN	22.285
220	C9 OLEFIN	22.332
221	C9 PARAFFIN	22.388
222	o-XYLENE	22.471
223	C9 PARAFFIN	22.558
224	1-NONENE	22.603
225	C9 PARAFFIN	22.655
226	C9 PARAFFIN	22.73
227	C9 PARAFFIN	22.81
228	n-NONANE	22.904
229	C10 PARAFFIN	23.044
230	C10 PARAFFIN	23.113
231	C10 PARAFFIN	23.175
232	ISOPROPYLBENZENE	23.325
233	C10 PARAFFIN	23.41
234	C10 PARAFFIN	23.505
235	C10 PARAFFIN	23.576
236	C10 PARAFFIN	23.694
237	C10 PARAFFIN	23.753
238	C10 PARAFFIN	23.81
239	a-PINENE	23.877
240	C10 OLEFIN	23.977
241	C10 PARAFFIN	24.047
242	n-PROPYLBENZENE	24.082
243	C10 PARAFFIN	24.18
244	m-ETHYLTOLUENE	24.256
245	p-ETHYLTOLUENE	24.317
246	C9 AROMATIC	24.448
247	4-METHYLNONANE	24.502
248	C10 PARAFFIN	24.564
249	o-ETHYLTOLUENE	24.722
250	C9 AROMATIC	24.849
251	C10 PARAFFIN	24.921
252	p,m,o-METHYLSTYRENE	24.992
253	1,2,4-TRIMETHYLBENZENE	25.087
254	C9 AROMATIC	25.19
255	C10 PARAFFIN	25.278
256	n-DECANE	25.39
257	C9 AROMATIC	25.467
258	sec-BUTYLBENZENE	25.531
259	C9 AROMATIC	25.64
260	1,2,3-TRIMETHYLBENZENE	25.779
261	1-METHYL-4-ISOPROPYLBENZENE	25.842
262	C11 PARAFFIN	25.913
263	C11 PARAFFIN	25.973
264	C10 AROMATIC	26.088
265	C10 AROMATIC	26.249
266	1,3-DIETHYLBENZENE	26.367
267	C10 AROMATIC	26.437

Table A.10, cont

268	1,4-DIETHYLBENZENE	26.58
269	C10 AROMATIC	26.677
270	1,2-DIETHYLBENZENE	26.712
271	C11 PARAFFIN	26.747
272	C10 AROMATIC	26.83
273	C11 PARAFFIN	26.893
274	C11 PARAFFIN	27.012
275	2,6-DIMETHYLSTYRENE	27.051
276	1,2-DIMETHYL-4-ETHYLBENZENE	27.097
277	C10 AROMATIC	27.233
278	C10 AROMATIC	27.291
279	C11 PARAFFIN	27.471
280	C10 AROMATIC	27.55
281	C10 AROMATIC	27.639
282	1,2-DIMETHYL-3-ETHYLBENZENE	27.679
283	C10 AROMATIC	27.823
284	1,2,4,5-TETRAMETHYLBENZENE	27.91
285	1,2,3,5-TETRAMETHYLBENZENE	27.986
286	C10 AROMATIC	28.063
287	ISOAMYLBENZENE	28.114
288	C10 AROMATIC	28.23
289	C9 PARAFFIN	20.633
290	C11 AROMATIC	28.493
291	C11 AROMATIC	28.532
292	C11 AROMATIC	28.6
293	C11 AROMATIC	28.715
294	1,2,3,4-TETRAMETHYLBENZENE	28.793
295	C11 AROMATIC	28.926
296	C11 AROMATIC	28.99
297	C11 AROMATIC	29.069
298	C11 AROMATIC	29.14
299	C11 AROMATIC	29.22
300	C11 AROMATIC	29.44
301	C11 AROMATIC	29.565
302	C11 AROMATIC	29.71
303	C11 AROMATIC	29.758
304	C12 PARAFFIN	29.809
305	C11 AROMATIC	29.947
306	C11 AROMATIC	30.029
307	C11 AROMATIC	30.08
308	C11 AROMATIC	30.153
309	C11 AROMATIC	30.237
310	C11 AROMATIC	30.468
311	C11 AROMATIC	30.597
312	C12 PARAFFIN	30.64
313	C11 AROMATIC	30.691
314	C12 AROMATIC	30.778
315	C12 AROMATIC	30.94
316	N-HEXYLBENZENE	31.032
317	C12 AROMATIC	31.123
318	C12 AROMATIC	31.175
319	C12 AROMATIC	31.253
320	C12 AROMATIC	31.341
321	C12 AROMATIC	31.487
322	C12 AROMATIC	31.537
323	C12 AROMATIC	31.794

Table A.10, cont

324	C12 AROMATIC	31.853
325	C12 AROMATIC	31.965
326	C12 AROMATIC	32.08
327	C12 AROMATIC	32.21
328	C13 PRAFFIN	32.25
329	C12 AROMATIC	32.4
330	C12 AROMATIC	32.493
331	C12 AROMATIC	32.588
332	C12 AROMATIC	32.693
333	C12 AROMATIC	32.793
334	C12 AROMATIC	32.93
335	C13 PARAFFIN	32.968
336	C12 AROMATIC	33.017
337	C12 AROMATIC	33.32
338	C12 AROMATIC	33.672
339	C12 AROMATIC	33.687
340	C12 AROMATIC	35.927
341	1&2-BUTYNE	7.21
342	C4 OLEFIN	8.097
343	C4 OLEFIN	8.22
344	C6 OLEFIN	13.543
345	C7 OLEFIN	15.363
346	C7 OLEFIN	16.026
347	C7 PARAFFIN	16.507
348	C7 OLEFIN	17.066
349	C8 OLEFIN	17.269
350	C8 OLEFIN	17.43
351	2,5-DIMETHYLHEXANE	18.13
352	C8 PARAFFIN	19.342
353	C8 PARAFFIN	19.933
354	C9 OLEFIN	20.413
355	C11 OLEFIN	27.357
356	C10 AROMATIC	27.42
357	C10 AROMATIC	28.375
358	C11 AROMATIC	30.177
359	C11 AROMATIC	30.314
360	C11 AROMATIC	30.53
361	C12 AROMATIC	30.85
362	C12 AROMATIC	31.622
363	C12 AROMATIC	31.747
364	C7 OLEFIN	15.487
365	C7 PARAFFIN	16.73
366	C8 PARAFFIN	17.95
367	C9 PARAFFIN	22.04
369	C6 PARAFFIN	13.18
370	C10 AROMATIC	28.84
371	C7 OLEFIN	14.89
372	C9 PARAFFIN	22.02
373	C10 AROMATIC	26.995
374	C10 AROMATIC	28.33
375	C4 OLEFIN	3.84
376	C6 OLEFIN	13.39
377	C11 AROMATIC	29.283
378	C12 AROMATIC	35.09
379	C11 AROMATIC	28.42
380	N-AMYLBENZENE	28.902

Table A.10, cont

381	C12 AROMATIC	33.246
382	C3 PARAFFIN	3.19
383	C3 PARAFFIN	4.3
384	C4 PARAFFIN	7.086
385	C6 PARAFFIN	12.279
386	C7 PARAFFIN	14.823
387	C7 OLEFIN	15.65
388	C8 PARAFFIN	19.02
389	C9 PARAFFIN	20.63
390	C12 AROMATIC	34.28
391	C4 PARAFFIN	7.45
392	C4 OLEFIN	8.72
393	C5 OLEFIN	9.57
394	C5 OLEFIN	9.99
395	C5 OLEFIN	11.66
396	C5 OLEFIN	12.02
397	C8 PARAFFIN	18.52
398	C9 PARAFFIN	21.33
399	C9 PARAFFIN	21.76
400	C10 PARAFFIN	23.64
401	C10 AROMATIC	26.5
402	C10 AROMATIC	27.18
403	C10 AROMATIC	27.72
404	C12 AROMATIC	32.33
405	C12 AROMATIC	34.46
406	C12 AROMATIC	35.74
407	C6 PARAFFIN	13.01
408	delta-3-CARENE	25.7
409	C11 AROMATIC	30.4
410	C12 AROMATIC	33.14
411	C12 AROMATIC	34.18
412	C5 OLEFIN	9.45
413	C5 OLEFIN	10.76
414	C12 AROMATIC	31.58
415	C7 OLEFIN	15.35
600	ETHYLENE + ACETYLENE	0
602	ETHYLENE	0
603	ACETYLENE	0
801	p-XYLENE	0
802	m-XYLENE	0

Table A.11. Assignment of EPA ambient data HC species to mechanisms species for CB4 and CAL mechanisms.

ID	Mechanism Species Name	Mechanism Species Carbon Number =>	c#Code	CB4 OLE 2	CB4 PAR 1	CB4 TOL 7	CB4 XYL 8	CB4 FORM 1	CB4 ALD2 2	CB4 ISOP 5	CB4 ETH 2	CB4 NR 1	CAL ETH 2	CAL PRPE 3	CAL TBUT 4	CAL ALK4 4.5	CAL ALK7 7	CAL TOLU 7	CAL XYLE 8	CAL TMB2 9	CAL HCHO 1	CAL ALD2 2	CAL RCHO 3	NR MISS 1
0	UNKNOWN		1 U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
101	ETHANE		2 P	0	0.4	0	0	0	0	0	0	1.6	0	0	0	0	0	0	0	0	0	0	1	1
102	ETHYLENE		2 O	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	1
103	ACETYLENE		2 Y	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0
104	PROPYLENE		3 O	1	1	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	1
105	PROPANE		3 P	0	1.5	0	0	0	0	0	0	1.5	0	0	0.5	0	0	0	0	0	0	0	0	0
106	UNKNOWN		1 U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	0.25	0
107	PARAFFIN		3 Q3	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
108	OLEFIN		4 R4	1	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-1.5	0
109	OLEFIN		4 R4	1	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0
110	ISOBUTANE		4 P	0	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
111	UNKNOWN		1 U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-0.5	0
112	UNKNOWN		1 U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-0.5	0
113	1-BUTENE		4 O	1	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0
114	1,3-BUTADIENE		4 D	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0
115	N-BUTANE		4 P	0	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
116	TRANS-2-BUTENE		4 O	0	0	0	0	0	2	0	0	0	0	1	0	1	0	0	0	0	0	0	-0.5	0
117	CIS-2-BUTENE		4 O	0	0	0	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
118	3-METHYL-1-BUTENE		5 O	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
119	ISOPENTANE		5 P	0	5	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0.5	0
120	C5 OLEFIN		5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
121	1-PENTENE		5 O	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
122	C5 OLEFIN		5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
123	2-METHYL-1-BUTENE		5 O	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
124	N-PENTANE		5 P	0	5	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	-2	0
125	ISOPRENE		5 D	2	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-2	1
126	TRANS-2-PENTENE		5 O	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
127	C5 OLEFIN		5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
128	2-METHYL-2-BUTENE		5 O	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	2
129	CIS-2-PENTENE		5 O	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
130	C5 OLEFIN		5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
131	C6 PARAFFIN		6 Q6	0	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	-1	0
132	C6 PARAFFIN		6 Q6	0	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	-1	0
133	2,2-DIMETHYLBUTANE		6 P	0	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	-1	0
134	C5 OLEFIN		5 R5	1	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1	0
135	C6 OLEFIN		6 R6	1	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	0
136	C6 PARAFFIN		6 Q6	0	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	-1	0
137	4-METHYL-1-PENTENE		6 O	1	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3	0
138	CYCLOPENTANE		5 E	0	5	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0.5	0
139	2,3-DIMETHYLBUTANE		6 P	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	-1

Table A.11, cont

	Mechanism Species Name =>		CB4									CAL												
	Mechanism Species Carbon Number =>		OLE 2	PAR 1	TOL 7	XYL 8	FORM 1	ALD2 2	ISOP 5	ETH 2	NR 1	ETH 2	PRPE 3	TBUT 4	ALK4 4.5	ALK7 7	TOLU 7	XYLE 8	TMBZ 9	HCHO 1	ALD2 2	RCHO 3	NR 1	MISS
ID	Name	c#Code																						
140	CIS-4-METHYL-2-PENTENE	6 O	0	2	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
140	CIS-4-METHYL-2-PENTENE	6 O	0	2	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
141	2-METHYLPENTANE	6 P	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1
142	TRANS-4-METHYL-2-PENTENE	6 O	0	2	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
143	C6 OLEFIN	6 R6	1	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3
144	C6 OLEFIN	6 R6	1	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3
145	3-METHYLPENTANE	6 P	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1
146	1-HEXENE	6 O	1	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3
147	C6 OLEFIN	6 R6	1	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3
148	N-HEXANE	6 P	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1
149	C7 PARAFFIN	7 Q7	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
150	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
151	2-METHYL-2-PENTENE	6 O	0	4	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
152	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
153	CIS-2-HEXENE	6 O	0	2	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
153	TRANS-2-HEXENE	6 O	0	2	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
153	2-HEXENE	6 O	0	2	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
154	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
155	3-METHYL-TRANS-2-PENTENE	6 O	0	4	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
156	METHYLCYCLOPENTANE	6 E	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1
157	2,4-DIMETHYLPENTANE	7 P	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
158	2,2,3-TRIMETHYL-1-BUTENE	7 O	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
159	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
160	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
161	C7 PARAFFIN	7 Q7	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
162	BENZENE	6 A	0	1	0	0	0	0	0	0	5	0	0	0	0	0.3	0	0	0	0	0	0	0.7	3.2
163	3,3-DIMETHYLPENTANE	7 P	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
163	CYCLOHEXANE	6 E	0	6	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
164	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
165	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
166	2-METHYLHEXANE	7 P	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
167	2,3-DIMETHYLPENTANE	7 P	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
168	CYCLOHEXENE	6 C	1	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
169	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
170	3-METHYLHEXANE	7 P	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
171	C7 PARAFFIN	7 Q7	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
172	C7 PARAFFIN	7 Q7	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
173	2,2,4-TRIMETHYLPENTANE	8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
173	ISOOCTANE	8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
174	CB OLEFIN	8 R8	1	6	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	5
175	N-HEPTANE	7 P	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
176	T-HEPTENE-2	7 O	0	3	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	3
177	CB OLEFIN	8 R8	1	6	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	5
178	C-HEPTENE-2	7 O	0	3	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	3
179	METHYLCYCLOHEXANE	7 E	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0

Table A.11, cont

ID	Mechanism Species Name	Mechanism Species Carbon Number =>	c#Code	-CB4- OLE 2	PAR 1	TOL 7	XYL 8	FORM 1	ALD2 2	ISOP 5	ETH 2	NR 1	-CAL- ETH 2	PRPE 3	TBUT 4	ALK4 4.5	ALK7 7	TOLU 7	XYLE 8	TMBZ 9	HCHO 1	ALD2 2	RCHO 3	NR 1	MISS
180	2,5-DIMETHYLHEXANE		8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
181	2,4-DIMETHYLHEXANE		8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
182	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
183	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
184	2,3,4-TRIMETHYLPENTANE		8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
185	TOLUENE		7 A	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
186	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
187	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
188	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
189	2-METHYLHEPTANE		8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
190	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
191	3-METHYLHEPTANE		8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
192	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
193	2,2,5-TRIMETHYLHEXANE		9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
194	1-OCTENE		8 O	1	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5
195	CYCLOHEPTANE		7 E	0	7	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	6
196	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	1
197	C8 PARAFFIN		8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	1
198	M-OCTANE		8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	1
199	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
200	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
201	C-2-OCTENE		8 O	0	4	0	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	5
202	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	6
203	C9 OLEFIN		9 R9	1	7	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2	6
204	2,4-DIMETHYLHEPTANE		9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
205	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
206	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
207	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
208	ETHYLCYCLOHEXANE		8 E	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	2
209	2,5-DIMETHYLHEPTANE		9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
210	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
211	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
212	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
213	ETHYLBENZENE		8 A	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	2
214	2,3-DIMETHYLHEPTANE		9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
215	M&P-XYLENE		8 A	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
216	4-METHYLOCTANE		9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
217	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
218	3-METHYLOCTANE		9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	2
219	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	6
220	C9 OLEFIN		9 R9	1	7	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2	6
221	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	1
222	O-XYLENE		8 A	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
223	C9 PARAFFIN		9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	6
224	1-NONENE		9 O	1	7	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2	6

Table A.11, cont

	Mechanism Species Name =>		CB4									CAL												
	Mechanism Species Carbon Number =>		OLE	PAR	TOL	XYL	FORM	ALD2	ISOP	ETH	NR	ETH	PRPE	TBUT	ALK4	ALK7	TOLU	XYLE	TMBZ	HCHO	ALD2	RCHO	NR	MISS
ID	Name	c#Code	2	1	7	8	1	2	5	2	1	2	3	4	4.5	7	7	8	9	1	2	3	1	
225	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
226	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
227	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
228	NONANE	9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
229	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
230	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
231	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
232	ISOPROPYLBENZENE	9 A	0	2	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
233	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2
234	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
235	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
236	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
237	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
238	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
239	A-PINENE	10 T	0.5	6	0	0	0	1.5	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	6
240	C10 OLEFIN	10 B10	1	8	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	7
241	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
242	N-PROPYLBENZENE	9 A	0	2	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2
243	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
244	M-ETHYLTOLUENE	9 A	0	1	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2
245	P-ETHYLTOLUENE	9 A	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
246	C9 AROMATIC	9 B9	0	1.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
247	4-METHYLNONANE	10 P	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	1.35
248	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
249	O-ETHYLTOLUENE	9 A	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
250	C9 AROMATIC	9 B9	0	1.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1
251	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	1.35
252	P-,M-,O-METHYLSTYRENE	9 A	0	1	1	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
253	1,2,4-TRIMETHYLBENZENE	9 A	0	1	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	7
254	C9 AROMATIC	9 B9	0	1.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
255	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	1.35
256	N-DECANE	10 P	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
257	C9 AROMATIC	9 B9	0	1.5	0.5	0.5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
258	SEC-BUTYLBENZENE	10 A	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	1.35
259	C9 AROMATIC	9 B9	0	1.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	3
260	1,2,3-TRIMETHYLBENZENE	9 A	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	1.35
261	1-METHYL-4-ISOPROPBENZE	10 A	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
262	C11 PARAFFIN	11 Q11	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
263	C11 PARAFFIN	11 Q11	0	11	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	4
264	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	4
265	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
266	1,3-DIETHYLBENZENE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
267	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
268	1,4-DIETHYLBENZENE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
269	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
												0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35

Table A.11, cont

ID	Mechanism Species Name => Mechanism Species Carbon Number => Name	c#Code	CB4 OLE 2	PAR 1	TOL 7	XYL 8	FORM 1	ALD2 2	ISOP 5	ETH 2	HR 1	ETH 2	PRPE 3	TBUT 4	CAL ALK4 4.5	ALK7 7	TOLU 7	XYLE 8	TMB2 9	HCHO 1	ALD2 2	RCHO 3	MR MISS 1
270	1,2-DIETHYLBENZENE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
271	C11 PARAFFIN	11 Q11	0	11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	4
272	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
273	C11 PARAFFIN	11 Q11	0	11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	4
274	C11 PARAFFIN	11 Q11	0	11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	4
275	2,6-DIMETHYLSTYRENE	10 A	0	1	1	0	0	1	0	0	0	0	1	0	0	0	0	0	1	0	0	0	8
276	DIMETHYLETHYLBENZENE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
277	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
278	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
279	C11 PARAFFIN	11 Q11	0	11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	4
280	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
281	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
282	1,2-DIMETHYL-3-ETHYLBENZE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
283	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
284	1,2,4,5-TETRAMETHYLBENZE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
285	1,2,3,5-TETRAMETHYLBENZE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
286	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
287	ISOAMYLBENZENE	11 A	0	4	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	4
288	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
289	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
290	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	0	2.5
291	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	0	2.5
292	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	0	2.5
293	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	0	2.5
294	1,2,3,4-TETRAMETHYLBENZE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
295	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
296	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
297	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
298	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
299	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
300	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
301	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
302	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
303	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
304	C12 PARAFFIN	12 Q12	0	12	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	5
305	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
306	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
307	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
308	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
309	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
310	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
311	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
312	C12 PARAFFIN	12 Q12	0	12	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	5
313	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
314	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5

Table A.11, cont

			CB4									CAL												
	Mechanism Species Name =>		OLE	PAR	TOL	XYL	FORM	ALD2	ISOP	ETH	NR	ETH	PRPE	TBUT	ALK4	ALK7	TOLU	XYLE	TMBZ	HCHO	ALD2	RCHO	NR	MISS
	Mechanism Species Carbon Number =>		2	1	7	8	1	2	5	2	1	2	3	4	4.5	7	7	8	9	1	2	3	1	
ID	Name	c#Code																						
315	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
316	N-HEXYLBENZENE	12 A	0	5	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	5
317	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
318	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
319	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
320	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
321	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
322	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
323	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
324	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
325	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
326	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
327	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
328	C13 PARAFFIN	13 Q13	0	13	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	6
329	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
330	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
331	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
332	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
333	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
334	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
335	C13 PARAFFIN	13 Q13	0	13	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	6
336	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
337	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
338	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
339	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
340	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
341	1&2 BUTYNE	4 Y	0	2	0	0	0	0	0	1	0	0.5	0	0	0.5	0	0	0	0	0	0	0	0	0.75
342	C4 OLEFIN	4 R4	1	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
343	C4 OLEFIN	4 R4	1	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
344	C6 OLEFIN	6 R6	1	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3
345	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
346	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
347	C7 PARAFFIN	7 Q7	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
348	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
349	C8 OLEFIN	8 R8	1	6	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	5
350	C8 OLEFIN	8 R8	1	6	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	5
351	2,5-DIMETHYLHEXANE	8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
352	C8 PARAFFIN	8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
353	C8 PARAFFIN	8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
354	C9 OLEFIN	9 R9	1	7	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	6
355	C11 OLEFIN	11 R11	1	9	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	8
356	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	3
357	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
358	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
359	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5

Table A.11, cont

			CB4									CAL												
Mechanism Species Name =>			OLE	PAR	TOL	XYL	FORM	ALD2	ISOP	ETH	NR	ETH	PRPE	TBUT	ALK4	ALK7	TOLU	XYLE	TMB2	HCHO	ALD2	RCHO	NR	MISS
Mechanism Species Carbon Number =>			2	1	7	8	1	2	5	2	1	2	3	4	4.5	7	7	8	9	1	2	3	1	
ID	Name	c#Code																						
360	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
361	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
362	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
363	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
364	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
365	C7 PARAFFIN	7 Q7	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
366	C8 PARAFFIN	8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
367	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
369	C6 PARAFFIN	6 Q6	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1
370	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
371	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
372	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
373	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
374	C10 AROMATIC	10 B10	0	2.5	0.5	0.5	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
375	C4 OLEFIN	4 R4	1	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
376	C6 OLEFIN	6 R6	1	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3
377	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
378	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
379	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
380	N-AMYLBENZENE	11 A	0	4	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	4
381	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
382	C3 PARAFFIN	3 Q3	0	3	0	0	0	0	0	0	0	0	0	0	0.5	0	0	0	0	0	0	0	0.5	0.25
383	C3 PARAFFIN	3 Q3	0	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-1.5
384	C4 PARAFFIN	4 Q4	0	4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-0.5
385	C6 PARAFFIN	6 Q6	0	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-1
386	C7 PARAFFIN	7 Q7	0	7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
387	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
388	C8 PARAFFIN	8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
389	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
390	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
391	C4 PARAFFIN	4 Q4	0	4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-0.5
392	C4 OLEFIN	4 R4	1	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
393	C5 OLEFIN	5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
394	C5 OLEFIN	5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
395	C5 OLEFIN	5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
396	C5 OLEFIN	5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
397	C8 PARAFFIN	8 Q8	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
398	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
399	C9 PARAFFIN	9 Q9	0	9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2
400	C10 PARAFFIN	10 Q10	0	10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
401	C10 AROMATIC	10 B10	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
402	C10 AROMATIC	10 B10	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
403	C10 AROMATIC	10 B10	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.35	0.15	0	0	0	0	2.35
404	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
405	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5

Table A.11, cont

	Mechanism Species Name =>																											
	Mechanism Species Carbon Number =>																											
						CB4													CAL									
			OLE	PAR	TOL	XYL	FORM	ALD2	ISOP	ETH	NR	ETH	PRPE	TBUT	ALK4	ALK7	TOLU	XYLE	TMBZ	HCHO	ALD2	RCHO	NR	MISS
			2	1	7	8	1	2	5	2	1	2	3	4	4.5	7	7	8	9	1	2	3	1	
ID	Name	c#Code																						
406	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
407	C6 PARAFFIN	6 Q6	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1
408	D-3-CARENE	10 T	2	6	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	6
409	C11 AROMATIC	11 B11	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	2.5
410	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
411	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0	0	0	0	3.5
412	C5 OLEFIN	5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
413	C5 OLEFIN	5 R5	1	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
414	C12 AROMATIC	12 B12	0	4	0	1	0	0	0	0	0	0	1	0	0	0	0	0.5	0.5	0	0	0	0	3.5
415	C7 OLEFIN	7 R7	1	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4
801	P-XYLENE	8 A	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
802	M-XYLENE	8 A	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
804	FORMALDEHYDE	1 L	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
805	ACETALDEHYDE	2 L	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
806	2-METHYL-1,3-BUTADIENE	5 D	2	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	3
807	PENTYNE	5 Y	0	5	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1
808	CYCLOPENTENE	5 C	1	3	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1
809	4-METHYLHEPTANE	8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1
810	2,2,3-TRIMETHYLPENTANE	8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1
811	2,3,3-TRIMETHYLPENTANE	8 P	0	8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	2
812	2,3,5-TRIMETHYLHEXANE	9 P	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	5
813	STYRENE	8 A	0	0	1	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1
814	1,3,5-TRIMETHYLBENZENE	9 A	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1
815	INDANE	9 A	0	9	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	3
816	BUTYLBENZENE	10 A	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1
817	TETRAMETHYLBENZENE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
818	UNKNOWNMSB	1 U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
819	UNKNOWNMSB	1 U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
820	NAPHTHALENE	10 A	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2
821	1-METHYLNAPHTHALENE	11 A	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

CLASS CODES:

U -- unknown
P -- alkanes
E -- cycloalkanes
O -- mono-alkenes
C -- cyclo-alkenes
D -- di-alkenes
Y -- alkynes
A -- aromatic
T -- terpenes
L -- aldehydes

Q -- unknown alkanes

R -- unknown alkenes

B -- unknown aromatics

B

Program Listing

Copies of the HC data files, HC speciation table, and the program sources and executable code for MS/PC-DOS machines are available on one high-density, 5.25 inch (AT-style) standard diskett for distribution costs.

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```
1  {$V-}{$R-}{$S-}
2  Program HCSplitPgm;
3   { Split *.HCC HC composition files for each year }
4  Uses
5   Crt,       {TP 4.0 fast screen io unit}
6   FileOpen, {Jeffries's standard file open and create unit}
7   ReadEtxt, {Jeffries's implementation of nested file io}
8   StrLib,    {useful string operations, eg, string to uppercase}
9   StrIO,     {procedures that allow read to work from strings}
10  EscChk,    {source of boolean Escape-key function}
11  ErrIO;     {Helps identify errors}
12
13 Const
14  title =     '          HC Composition Fractions For CB4 and CAL Mechanisms.';
15  copyright = '      Copyright, (c) H.E. Jeffries and K.G. Sexton, 1988';
16  version   = '                    Version Sept. 4, 1988';
17
18  stop          = true;
19  showfile      = true;
20  noshow        = false;
21
22 Type
23  float        = double;
24
25 VAR
26  i,j,l         : integer;
27
28  CmdLine : string;
29  Command : string[4];
30
31  todays_date, todays_time: DTstring;
32
33  DataDefaultdir,
34  SpltDefaultdir,
35  ErrFileName,
36  SPLTFileName,
37  GenFileName, switches : filenamestring;
38
39  InFile  : EText;
40  Ifile   : PtrText;
41  OutFile : text;
42  obuf    : array[1..1024] of char;
43  ErrFile : text;
44
45  {Variables for processing }
46 const
47   MaxSpecies=350;
48   IDLength=4;
49   IDStringLen=1400; {IDLength*MaxSpecies}
50   MaxNumCorr=30;
51   HCNameLen =30;
52 Type
53   cb4species =(eth,ole,par,tol,xyl,nr,form,ald,un);
54   calspecies=(_eth,_prpe,_tbut,_alk4,_alk7,_tol,_xyl,_tmb,
55               _nr,_form,_ald,_rcho,_miss,_un);
56
57    {species fraction arrays}
58    Cfarray = array[ eth .. un] of float;
59    Lfarray = array[_eth .._un] of float;
60    {unknown, but classified compounds}
61   uCfarray = array[ ole .. nr] of float;
62   uLfarray = array[_prpe.._nr] of float;
63    {missing carbon by class}
64   mLfarray = array[_prpe.._nr] of float;
65
66
```

```
67    IDstring = string[IDLength];
68    SpNameString= string[4];
69    CIdStr  = string[4];
70    CanIDstr= string[6];
71    YYstr   = string[2];
72
73    Splitline=
74     record
75      name:string[HCNameLen];
76      cn:integer;
77      hctype:char;
78      cb4frac: array[ eth.. ald ] of single;
79      calfrac: array[_eth.._miss] of single;
80     end;
81
82  Var
83    HCid    : array[0..IDStringLen] of char;
84    HCSplit : array[1..MaxSpecies]  of SplitLine;
85    HCHeader: string; {file ID string}
86
87    {Carbon Numbers of each mechanism species}
88    CarNCB4 : Cfarray;
89    CarNCAL : Lfarray;
90    {Names of each mechanism species}
91    NameCB4 : array[ eth.. un] of SpNameString;
92    NameCAL : array[_eth.._un] of SpNameString;
93
94    {total set accumulators}
95     TotCB4f:  Cfarray;
96    uTotCB4f: uCfarray;
97     TotCALf:  Lfarray;
98    uTotCALf: uLfarray;
99    mTotCALf: mLfarray;
100
101   TotCount : integer;
102   TotNMHC, TotCNMHC, TotLNMHC: float;
103
104   {cluster accumulators}
105    CluCB4f:  Cfarray;
106   uCluCB4f: uCfarray;
107    CluCALf:  Lfarray;
108   uCluCALf: uLfarray;
109   mCluCALf: mLfarray;
110
111   CluCount : integer;
112   CluNMHC, CluCNMHC, CluLNMHC: float;
113
114   {file accumulators}
115    FilCB4f:  Cfarray;
116   uFilCB4f: uCfarray;
117    FilCALf:  Lfarray;
118   uFilCALf: uLfarray;
119   mFilCALf: mLfarray;
120
121   FilCount : integer; {number of cans in a file}
122   FilNMHC, FilCNMHC, FilLNMHC: float;
123
124   {single can accumulators}
125    CanCB4f:  Cfarray;
126   uCanCB4f: uCfarray;
127    CanCALf:  Lfarray;
128   uCanCALf: uLfarray;
129   mCanCALf: mLfarray;
130
131   CanCount : integer; {needed for general calls to routines}
132   CanNMHC, CanCNMHC, CanLNMHC: float;
```

```
133
134     CCity  : CIdstr;
135     CanId,
136      OldCanId: CanIDstr;
137     YY     : YYStr;
138
139     SplitFileRead : boolean;
140     PrintEachCan, PrintMiss, PrintUnkn : boolean;
141
142     LineCount,UseLineCount: integer;
```

```
143 {<f>}
144 Procedure Sig_Error(mess:string; showfile, action:boolean);
145  var
146   i: integer;
147   line: string;
148   oldattr: integer;
149  begin
150   OldAttr:=TextAttr;
151   TextColor(Red);
152   Writeln('ERROR:::',mess);
153   if showfile
154    then
155     begin
156      writeln('Next 3 lines were:');
157      TextColor(Yellow);
158      for i:= 1 to 3 do
159       if not eof(Ifile^)
160        then
161         begin
162          readln(Ifile^,line);
163          writeln(line);
164         end;
165     end;
166   TextAttr:=OldAttr;
167   if action then halt(7);
168  end;
169
170 {$F+}
171 Procedure ErrCloseFiles;
172  begin
173   if FileOpened(OutPut) then Close(OutPut);
174  end;
175 {$F-}
```

```
176 {<f>}
177  Procedure HeaderOut; forward;
178  Procedure LoadHCSplit(HCFname: filenamestring);
179  var
180   HCFile: text;
181   hbuf  : array[1..1024] of char;
182   i, k  : integer;
183   id    : IDstring;
184   d     : char;     {1 blank}
185   d5    : string[5];{5 blanks}
186   cs    : cb4species;
187   ls    : calspecies;
188  begin
189   if NOT SetUpFile(wherey,HCFname,HCFile,'R',hbuf,sizeof(hbuf))
190    then Sig_Error('Can Not Locate HC Data File '+HCFname+'.',noshow,stop);
191   readln(HCFile,HCHeader);
192   Writeln(OutFile, 'Data Processed on ',todays_date,' at ',todays_time,
193                    ' using species splits file:');
194   Writeln(OutFile,HCHeader);
195   with HCSplit[1] do
196    begin
197     read(HCFile, d,name,cn,d,d,d);  {dummy position holding data}
198     for cs:= eth to  ald  do read(HCFile,d,NameCB4[cs]);
199     read(HCFile,d5);
200     for ls:=_eth to _miss do read(HCFile,d,NameCAL[ls]);
201     readln(HCFile);
202     read(HCFile, d,name,cn,d,d,d);  {dummy position holding data}
203     for cs:= eth to  ald  do read(HCFile,d,CarNCB4[cs]);
204     for ls:=_eth to _miss do read(HCFile,d,CarNCAL[ls]);
205     readln(HCFile);
206     NameCB4[ un]:='UNKN';
207     NameCAL[_un]:='UNKN';
208     CarNCB4[ un]:=1.0;
209     CarNCAL[_un]:=1.0;
210    end;
211   i:=1;
212   k:=1;
213   while (NOT eof(HCFile) and (i<MaxSpecies)) do
214    begin
215     {add id to end of long string}
216     read(HCFile,id);
217     Move(id[1],HCid[k],4);
218     with HCSplit[i] do
219      begin
220       read(HCFile, d,name,cn,d,hctype,d,d,d);
221       for cs:= eth to  ald  do read(HCFile,cb4frac[cs]);
222       for ls:=_eth to _miss do read(HCFile,calfrac[ls]);
223       readln(HCFile);
224      end;
225     inc(i);
226     k:=IDLength*(i-1)+1;
227    end;
228   Writeln('HC Splits file loaded...');
229   HeaderOut;
230   SplitFileRead:=true;
231  end;
```

```
232 (<f>)
233  Function FindID(Id:Idstring; Var Index:integer):boolean;
234   begin
235    Index:=(LongPosFwd__(HCid,1,IDStringLen,Id)+sizeof(Id)-2) div (sizeof(Id)-1);
236    if (Index>0) and (Index<=MaxSpecies)
237     then FindID:=true
238     else FindID:=false;
239   end;
240
241  Procedure ZeroAcc(Var  CB4f:  Cfarray;
242                    Var uCB4f: uCfarray;
243                    Var  CALf:  Lfarray;
244                    Var uCALf: uLfarray;
245                    Var mCALf: mLfarray;
246                    Var Count: integer;
247                    Var NMHC : float);
248   var
249    cs : cb4species;
250    ls : calspecies;
251   begin
252    For cs:=  eth  to  un  do  CB4f[cs]:=0.0;
253    For ls:= _eth  to _un  do  CALf[ls]:=0.0;
254    For cs:=  ole  to  nr  do uCB4f[cs]:=0.0;
255    For ls:= _prpe to _nr  do
256     begin
257      uCALf[ls]:=0.0;
258      mCALf[ls]:=0.0;
259     end;
260    Count:=0;
261    NMHC:=0.0;
262   end;
263
264 Procedure SpeciateConc(J:integer; amt: float);
265  { j   is index of HCdata table for compound,
266    amt is the ppbC of compound in canister.}
267  Const
268   cb4unktype : array[ole..nr] of char
269                = ('R','Q','B','B',' ');
270                  {ole,par,tol,xyl,nr}
271   calunktype : array[_prpe.._nr] of char
272                = ('R', 'R', 'Q', 'Q', 'B', 'B', 'B', ' ');
273                  {prpe tbut alk4 alk7 tol  xyl  tmb   nr}
274   calmisstype: array[_prpe.._nr] of string[10]
275                = (( _prpe) 'ABCOR',
276                   ( _tbut) 'CDORT',
277                   ( _alk4) 'EPQ',
278                   ( _alk7) 'ABEPQ',
279                   ( _tol ) 'AB',
280                   ( _xyl ) 'AB',
281                   ( _tmb ) 'AB',
282                   ( _nr  ) 'ABCDEPQORY');
283  var
284   t: char;
285   cs : cb4species;
286   ls : calspecies;
287   missamt: float;
288  begin
289   with HCSplit[J] do
290    begin
291     amt:=amt/cn;
292     t:=HCtype;
293     if (t='U')
294      then
295       begin
296        CanCB4f[ un]:=CanCB4f[ un]+amt;
297        CanCALf[_un]:=CanCALf[_un]+amt;
```

```
298         end
299        else
300         begin
301          for cs:=eth to ald do
302           if (cb4frac[cs]>0)
303            then CanCB4f[cs]:=CanCB4f[cs]+amt*cb4frac[cs];
304          for ls:=_eth to _miss do
305           if (calfrac[ls]<>0.0)
306            then CanCALf[ls]:=CanCALf[ls]+amt*calfrac[ls];
307          { track composition of speciated unknowns)
308          for cs:=ole to nr do
309          if ((t=cb4unktype[cs])  and (cb4frac[cs]>0))
310           then uCanCB4f[cs]:=uCanCB4f[cs]+amt*cb4frac[cs];
311          for ls:=_prpe to _nr do
312          if ((t=calunktype[ls])  and (calfrac[ls]>0))
313           then uCanCALf[ls]:=uCanCALf[ls]+amt*calfrac[ls];
314          { track composition of missing fraction for CAL)
315          missamt:=amt*calfrac[_miss];
316          for ls:=_prpe to _nr do
317           if ((CanCALf[ls]>0) and (pos(t,calmisstype[ls])>0) and (calfrac[ls]>0))
318            then mCanCALf[ls]:=mCanCALf[ls]+missamt*calfrac[ls];
319         end;
320     end; (with )
321   end;
322
323   Procedure AddOneCan(Var  CB4f:  Cfarray;
324                       Var uCB4f: uCfarray;
325                       Var  CALf:  Lfarray;
326                       Var uCALf: uLfarray;
327                       Var mCALf: mLfarray;
328                       Var Count: integer;
329                       Var NMHC : float);
330    var
331     cs: cb4species;
332     ls: calspecies;
333    begin
334     for cs:= eth  to  un do  CB4f[cs]:= CB4f[cs]+ CanCB4f[cs];
335     for ls:=_eth  to _un do  CALf[ls]:= CALf[ls]+ CanCALf[ls];
336     for cs:= ole  to  nr do uCB4f[cs]:=uCB4f[cs]+uCanCB4f[cs];
337     for ls:=_prpe to _nr do uCALf[ls]:=uCALf[ls]+uCanCALf[ls];
338     for ls:=_prpe to _nr do mCALf[ls]:=mCALf[ls]+mCanCALf[ls];
339     Count:=Count+1;
340     NMHC :=NMHC +CanNMHC;
341   end;
342
343  Procedure CalcFrac(Var  CB4f:  Cfarray;
344                     Var uCB4f: uCfarray;
345                     Var  CALf:  Lfarray;
346                     Var uCALf: uLfarray;
347                     Var mCALf: mLfarray;
348                         Count: integer;
349                     Var NMHC, CNMHC, LNMHC : float);
350   var
351    cs: cb4species;
352    ls: calspecies;
353   begin
354    CNMHC:=0.0;
355    LNMHC:=0.0;
356    (compute total NMHC for each mechanism)
357    for cs:= eth  to  un do
358     begin
359      CB4f[cs]:= CB4f[cs]*CarNCB4[cs];
360      CNMHC:=CNMHC+CB4f[cs];
361     end;
362    for ls:=_eth  to _un do
363     begin
```

```
364       CALf[ls]:= CALf[ls]*CarNCAL[ls];
365       LNMHC:=LNMHC+CALf[ls];
366      end;
367    {compute class fractions }
368    for cs:= eth  to  un do  CB4f[cs]:= CB4f[cs]/CNMHC;
369    for ls:=_eth  to _un do  CALf[ls]:= CALf[ls]/LNMHC;
370
371    for cs:= ole  to  nr do uCB4f[cs]:=(uCB4f[cs]*CarNCB4[cs])/CNMHC;
372    for ls:=_prpe to _nr do uCALf[ls]:=(uCALf[ls]*CarNCAL[ls])/LNMHC;
373    for ls:=_prpe to _nr do mCALf[ls]:=(mCALf[ls]*CarNCAL[ls])/LNMHC;
374
375     NMHC:= NMHC/Count;
376    CNMHC:=CNMHC/Count;
377    LNMHC:=LNMHC/Count;
378   end;
379
380  Procedure HeaderOut;
381   var
382    cs: cb4species;
383    ls: calspecies;
384   begin
385    write(outfile,'City Yr ');
386    if PrintEachCan
387     then write(outfile,'CanID  NMHC  ')
388     else write(outfile,'NoSam  NMHC  ');
389    for cs:= eth  to un  do write(outfile,'  ',NameCB4[cs]:4);
390    write(outfile,' CB4HC');
391    for ls:= _eth to _un do write(outfile,'  ',NameCAL[ls]:4);
392    write(outfile,' CALHC');
393    if PrintMiss
394     then for ls:= _prpe to _nr do write(outfile,' M',NameCAL[ls]:4);
395    if PrintUnkn
396     then
397      begin
398       for cs:=  ole  to  nr do write(outfile,' U',NameCB4[cs]:4);
399       for ls:= _prpe to _nr do write(outfile,' U',NameCAL[ls]:4);
400      end;
401    writeln(outfile);
402   end;
403
404   Procedure DataOut(Var  CB4f:  Cfarray;
405                     Var uCB4f: uCfarray;
406                     Var  CALf:  Lfarray;
407                     Var uCALf: uLfarray;
408                     Var mCALf: mLfarray;
409                         Count: integer;
410                         CanId: CanIDstr;
411                         CityId: CIdstr;
412                         YY   : YYstr;
413                     Var NMHC, CNMHC, LNMHC : float);
414   var
415    cs: cb4species;
416    ls: calspecies;
417   begin
418    if (LineCount=UseLineCount)
419     then
420      begin
421       writeln(outfile,#12#10#10{FF,LF,LF}); {Top of new page}
422       HeaderOut;
423       LineCount:=1;
424      end
425     else
426      inc(LineCount);
427    write(outfile,CityId,' ',YY,' ');
428    if PrintEachCan
429     then write(outfile, CanId:6,' ',NMHC:5:0,' ')
```

```
430     else write(outfile, Count:6,' ',NMHC:5:0,' ');
431    for cs:= eth  to un  do write(outfile,CB4f[cs]:6:3);
432    write(outfile,CNMHC:6:0);
433    for ls:= _eth to _un do write(outfile,CALf[ls]:6:3);
434    write(outfile,LNMHC:6:0);
435    if PrintMiss
436     then for ls:= _prpe to _nr do write(outfile,mCALf[ls]:6:3);
437    if PrintUnkn
438     then
439      begin
440       for cs:=  ole  to  nr do write(outfile,uCB4f[cs]:6:3);
441       for ls:= _prpe to _nr do write(outfile,uCALf[ls]:6:3);
442      end;
443    writeln(outfile);
444   end;
445
446   Procedure ProcessACan;
447    begin
448     AddOneCan(FilCB4f,uFilCB4f,FilCALf,uFilCALf,mFilCALf,FilCount,FilNMHC);
449     AddOneCan(CluCB4f,uCluCB4f,CluCALf,uCluCALf,mCluCALf,CluCount,CluNMHC);
450     AddOneCan(TotCB4f,uTotCB4f,TotCALf,uTotCALf,mTotCALf,TotCount,TotNMHC);
451     If PrintEachCan
452      then
453       begin
454        CalcFrac(CanCB4f,uCanCB4f,CanCALf,uCanCALf,mCanCALf,1,
455                                        CanNMHC,CanCNMHC,CanLNMHC);
456
457        DataOut(CanCB4f,uCanCB4f,CanCALf,uCanCALf,mCanCALf,
458                    1, OldCanId, CCity,YY,CanNMHC,CanCNMHC,CanLNMHC);
459       end;
460     ZeroAcc(CanCB4f,uCanCB4f,CanCALf,uCanCALf,mCanCALf,CanCount,CanNMHC);
461    end;
462
463   Procedure ProcessAFile;
464    var
465     d: char; {1 blank}
466     Conc   : single;
467     GoodID : boolean;
468     SpId   : IDstring;
469     rest   : string[80];
470     Ifile  : PtrText;
471    begin
472     OldCanID:='';
473     Ifile:=Cvt(InFile);
474     {read the city and year from first line of file}
475     readln(Ifile^,CCity,rest);
476     YY:=copy(rest,pos('19',rest)+2,2);
477     repeat
478      readln(Ifile^, CanId,Conc,d,SpId);
479      if OldCanID='' then OldCanID:=CanId; {handle first data line in file}
480      GoodID:=true;
481      If Not FindId(SpId,J)
482       then
483        begin
484         if not FileOpened(ErrFile)
485          then if NOT SetUpFile(wherey,ErrFileName,ErrFile,'W',NONE_,0)
486           then Sig_Error('Can not open ERROR File.',noshow,stop);
487         writeln(ErrFile, 'Species not found in HCSplit File:');
488         writeln(ErrFile, CCity,' ',CanId,' ',Conc:8:1,' ',SpId:4);
489         writeln(ErrFile);
490         GoodID:=false;
491        end
492       else
493        begin
494         CanNMHC:=CanNMHC+Conc;
495         if CanId<>OldCanId
```

```
496          then
497           begin
498            ProcessACan;
499            OldCanId:=CanId;
500            SpeciateConc(J,Conc);{the first species in this can}
501           end
502          else
503           SpeciateConc(J,Conc); {rest of species in a can}
504        end;
505     until eof(Ifile^);
506     OldCanId:=CanId;
507     if GoodID then SpeciateConc(J,Conc);{last species in last can}
508     ProcessACan; {do last CanID}
509     {then calc and print whole file and zero acc}
510     if PrintEachCan then writeln(OutFile);
511     CalcFrac(FilCB4f,uFilCB4f,FilCALf,uFilCALf,mFilCALf,FilCount,
512                                   FilNMHC,FilCNMHC,FilLNMHC);
513     DataOut(FilCB4f,uFilCB4f,FilCALf,uFilCALf,mFilCALf,
514                  FilCount, '      ', CCity,YY,FilNMHC,FilCNMHC,FilLNMHC);
515     ZeroAcc(FilCB4f,uFilCB4f,FilCALf,uFilCALf,mFilCALf,FilCount,FilNMHC);
516     if PrintEachCan then begin writeln(OutFile); writeln(OutFile); end;
517    end;
518
519   Procedure ProcessACluster;
520    begin
521     writeln(OutFile,'For Cluster ',copy(CmdLine,pos('=',CmdLine)+1,length(CmdLine)));
522     CalcFrac(CluCB4f,uCluCB4f,CluCALf,uCluCALf,mCluCALf,CluCount,
523                                   CluNMHC,CluCNMHC,CluLNMHC);
524     DataOut(CluCB4f,uCluCB4f,CluCALf,uCluCALf,mCluCALf,
525                  CluCount, 'SubTot', '    ',' ',CluNMHC,CluCNMHC,CluLNMHC);
526     ZeroAcc(CluCB4f,uCluCB4f,CluCALf,uCluCALf,mCluCALf,CluCount,CluNMHC);
527     writeln(OutFile);
528    end;
529
530   Procedure ProcessTotal;
531    begin
532     if TotCount>0 then
533      begin
534     writeln(OutFile);
535     writeln(OutFile);
536     writeln(OutFile,'Total for all canisters ');
537     CalcFrac(TotCB4f,uTotCB4f,TotCALf,uTotCALf,mTotCALf,TotCount,
538                                   TotNMHC,TotCNMHC,TotLNMHC);
539     DataOut(TotCB4f,uTotCB4f,TotCALf,uTotCALf,mTotCALf,
540                  TotCount, 'Total', '    ',' ',TotNMHC,TotCNMHC,TotLNMHC);
541     writeln(OutFile);
542     end;
543    end;
544
545   Procedure FileCmd;
546    var
547     line:string;
548    begin
549     if NOT SplitFileRead
550      then
551       begin
552        GenFileName:=AddBackSlash_(SPLTDefaultDir)+SpltFileName;
553        LoadHCSplit(GenFileName);
554       end;
555     GenFileName:=copy(CmdLine,pos('=',CmdLine)+1,length(CmdLine));
556     if (length(DataDefaultdir) <> 0)
557      then GenFileName:=AddBackSlash_(DataDefaultdir)+GenFileName;
558     if NOT FileExists(GenFileName)
559      then Sig_Error('Can not find file '+GenFileName,noshow,stop);
560     ResetEText(InFile, GenFileName, EchoOff);
561     ProcessAFile;
```

```
562     writeln('File '+GenFileName+' processed...');
563     CloseEText(InFile);
564   end;
565
```

```
566  {<f>}
567   Procedure InitVar;
568    begin
569     FillChar(HCid,IDStringLen+1,' ');
570     DataDefaultdir:='';
571     SpltDefaultdir:=PgmRunPath_; {automatically set in FileOpen}
572     SpltFileName:='SpecSplt.dat';{can be changed by command}
573     SplitFileRead:=false;
574     ErrFileName:=GetOpenFileName(Cvt(InFile)^);
575     AddNewExt__('ERR',ErrFileName);
576     ZeroAcc(TotCB4f,uTotCB4f,TotCALf,uTotCALf,mTotCALf,
577                     TotCount,TotNMHC);
578     ZeroAcc(CluCB4f,uCluCB4f,CluCALf,uCluCALf,mCluCALf,
579                     CluCount,CluNMHC);
580     ZeroAcc(FilCB4f,uFilCB4f,FilCALf,uFilCALf,mFilCALf,
581                     FilCount,FilNMHC);
582     ZeroAcc(CanCB4f,uCanCB4f,CanCALf,uCanCALf,mCanCALf,
583                     CanCount,CanNMHC);
584     GetDateStr(todays_date);
585     GetTimeStr(todays_time);
586     LineCount:=0;
587    end;
588
589   Procedure Help;
590    begin
591     writeln('Expected Command Line Input:');
592     writeln(' HCSplit  cmd_file_name  out_file_name[/s/s/s]');
593     writeln('   where /s is one of:');
594     writeln('    /C -- print data for each can (can be >772 lines!)');
595     writeln('    /U -- add speciated unknowns to output.');
596     writeln('    /M -- add speciated MISS to output.');
597     writeln('    /Lnn -- change lines per page to nn.');
598     writeln;
599    end;
```

```
600  (<f>)
601  begin  { main }
602   InitErrIO(@ErrCloseFiles);
603   TextBackground(Black);
604   ClrScr;
605   TextColor(Yellow);
606   writeln(title);
607   TextColor(Red);
608   writeln(copyright);
609   TextColor(Green);
610   writeln(version);
611   writeln;
612   if ParamCount<1 then Help;
613   TextColor(LightCyan);
614
615   (Extended Text pointer should be initialized before first call)
616   InFile := InitEText;
617   if ParamCount >= 1
618    then GenFileName := ParamStr(1)
619    else GenFileName := '';
620   OpenEText(InFile, 'Enter name of command file ',GenFileName,switches);
621   if ParamCount >= 2
622    then GenFileName := ParamStr(2)
623    else GenFileName := '';
624   OpenFile(OutFile, 'Enter name of  output file ',GenFileName,switches,
625                 obuf, sizeof(obuf),'W');
626
627   if pos('/C',switches)<>0
628    then PrintEachCan:=true
629    else PrintEachCan:=false;
630
631   if pos('/U',switches)<>0
632    then PrintUnkn:=true
633    else PrintUnkn:=false;
634
635   if pos('/M',switches)<>0
636    then PrintMiss:=true
637    else PrintMiss:=false;
638
639   i:=pos('/L',switches);
640   if (i<>0)
641    then UseLineCount:=GetAnInteger(switches,i+2)
642    else UseLineCount:=48; {landscape at 8/in=7inches}
643
644   Window(1,5,79,25);
645   TextColor(White);
646   ClrScr;
647   InitVar;
648
649   repeat
650    readln(Ext(InFile)^,CmdLine);
651    Command:=StrUp(copy(CmdLine,1,4));
652    writeln(CmdLine);
653    if (Command='FILE') then FileCmd
654    else
655    if (Command='CLUS') then ProcessACluster
656    else
657    if (Command='EXIT') then ProcessTotal
658    else
659    if (Command='SPLT')
660     then SPLTDefaultdir:=copy(CmdLine,pos('=',CmdLine)+1,length(CmdLine))
661    else
662    if (Command='SPLI')
663     then SPLTFileName:=copy(CmdLine,pos('=',CmdLine)+1,length(CmdLine))
664    else
665    if (Command='DATA')
```

```
666      then DataDefaultdir:=copy(CmdLine,pos('=',CmdLine)+1,length(CmdLine))
667     else
668     if (length(CmdLine)=0)
669      then { blank line --- just skip it }
670     else
671      writeln('Unknown Command.');
672    until (Command='EXIT');
673
674    CloseEText(InFile);
675    Close(OutFile);
676    if FileOpened(ErrFile)
677     then
678      begin
679       writeln(^G^G'There were errors. See Error File.');
680       close(ErrFile);
681      end;
682    writeln;
683    writeln('Finished.');
684   end.
```

_ald 1.55
_alk4 1.54
_alk7 1.54
_eth 1.54 1.59 5.200 5.204 5.222 6.253 7.304 7.335 7.362 8.369
8.391 9.433
_eth.._miss 2.79
_eth.._un 2.92
_form 1.55
_miss 1.55 5.200 5.204 5.222 7.304 7.315
_nr 1.55 6.255 7.311 7.316 7.337 7.338 8.372 8.373 8.394 8.399
9.436 9.441
_prpe 1.54 6.255 7.311 7.316 7.337 7.338 8.372 8.373 8.394 8.399
9.436 9.441
_prpe.._nr 1.62 1.64 6.271 6.274
_rcho 1.55
_tbut 1.54
_tmb 1.54
_tol 1.54
_un 1.55 5.207 5.209 6.253 6.297 7.335 7.362 8.369 8.391 9.433
_xyl 1.54
.. 1.58 1.61
.._un 1.59
AddOneCan <7.323 9.448 9.449 9.450
ald 1.53 2.78 5.198 5.203 5.221 7.301
Black 13p603
CalcFrac <7.343 9.454 10.511 10.522 10.537
CanCALf 2.127 6.297 7.306 7.317 7.335 9p454 9p457 9p460 12p582
CanCB4f 2.125 6.296 7.303 7.334 9p454 9p457 9p460 12p582
CanCNMHC 2.132 9p455 9p458
CanCount 2.131 9p460 12p583
CanIDstr 2.70 3.136 8.410
CanId 3.135 8.410 8.429 9p478 9.479 9p488 9.495 10.499 10.506
CanLNMHC 2.132 9p455 9p458
CanNMHC 2.132 7.340 9p455 9p458 9p460 9=494 12p583
CarNCAL 2.89 5.204 5.209 8.364 8.372 8.373
CarNCB4 2.88 5.203 5.208 7.359 8.371
CCity 3.134 9p458 9p475 9p488 10p514
Cfarray 1.58 2.88 2.95 2.105 2.115 2.125 6.241 7.323 7.343 8.404
CIdStr 2.69
CIdstr 3.134 8.411
Close 14.675
CloseEText 14.674
ClrScr 13.604 13.646
CluCALf 2.107 9p449 10p522 10p524 10p526 12p578
CluCB4f 2.105 9p449 10p522 10p524 10p526 12p578
CluCNMHC 2.112 10p523 10p525
CluCount 2.111 9p449 10p522 10p525 10p526 12p579
CluLNMHC 2.112 10p523 10p525
CluNMHC 2.112 9p449 10p523 10p525 10p526 12p579
CmdLine 1.28 10p521 10p555 13p650 13p651 13p652 13p660 13p663 14p666 14p668
Command 1.29 13=651 13.653 13.655 13.657 13.659 13.662 13.665 14.672
Crt 1.5
calfrac 2.79 5.222 7.305 7.306 7.312 7.313 7.315 7.317 7.318
calspecies 1.54 5.187 6.250 6.286 7.332 7.352 8.383 8.416
cb4frac 2.78 5.221 7.302 7.303 7.309 7.310
cb4species 1.53 5.186 6.249 6.285 7.331 7.351 8.382 8.415
cn 2.76 5p197 5p202 5p220 6.291
copyright 1.15 13p608
DataDefaultdir 1.33 10p556 10p557 12=570 14=666
DataOut <8.404 9.457 10.513 10.524 10.539
DTstring 1.31

double 1.23
ErrCloseFiles <4.171 13.602
ErrFile 1.43 9p484 9p485 9p487 9p488 9p489 14p676 14p680
ErrFileName 1.35 9p485 12=574 12p575
ErrIO 1.11
EscChk 1.10
EText 1.39
eth 1.53 1.58 5.198 5.203 5.221 6.252 7.301 7.334 7.357 8.368
8.389 9.431
eth.. 2.78 2.91
FilCALf 2.117 9p448 10p511 10p513 10p515 12p580
FilCB4f 2.115 9p448 10p511 10p513 10p515 12p580
FilCNMHC 2.122 10p512 10p514
FilCount 2.121 9p448 10p511 10p514 10p515 12p581
FileCmd <10.545 13.653
FileOpen 1.6
FileOpened 14.676
FilLNMHC 2.122 10p512 10p514
FilNMHC 2.122 9p448 10p512 10p514 10p515 12p581
FindID <6.233 6=237 6=238
filenamestring 1.37 5.178
float 1.23 1.58 1.59 1.61 1.62 1.64 2.102 2.112 2.122 2.132
6.247 6.264 6.287 7.329 7.349 8.413
form 1.53
GenFileName 1.37 10=552 10p553 10=555 10=557 10p558 10.559 10p560 11.562
13=618 13=619 13p620 13=622 13=623 13p624
GetAnInteger 13.641
Green 13p609
HCHeader 2.85 5p191 5p194
HCid 2.83 5.217 6p235 12p569
HCNameLen 1.51 2.75
HCSplit 2.84 5.195 5.218 6.289
HCSplitPgm 1.2
HeaderOut <5.177 <8.380 5.229 8.380 8.422
Help <12.589 13.612
hctype 2.77 5p220
IDLength 1.48 2.67 5.226
IDStringLen 1.49 6p235 12.569
IDstring 2.67 5.183 9.468
Ifile 1.40 4.159 4.162 9.470 9=473 9.475 9.478 10.505
InFile 1.39 9p473 10p560 11p563 12p574 13=616 13p620 13p650 14p674
InitErrIO 13.602
InitEText 13.616
InitVar <12.567 13.647
i 1.26 4.146 4=158 5.182 5=211 5.213 5.218 5p225 5.226 13=639
13.640 13.641
j 1.26
Lfarray 1.59 2.89 2.97 2.107 2.117 2.127 6.243 7.325 7.345 8.406
LightCyan 13p613
LineCount 3.142 8.418 8=423 8p426 12=586
LoadHCSplit <5.178 10.553
l 1.26
MaxNumCorr 1.50
MaxSpecies 1.47 5.213 6.236
mCanCALf 2.129 7.318 7.338 9p454 9p457 9p460 12p582
mCluCALf 2.109 9p449 10p522 10p524 10p526 12p578
mFilCALf 2.119 9p448 10p511 10p513 10p515 12p580
mLfarray 1.64 2.99 2.109 2.119 2.129 6.245 7.327 7.347 8.408
mTotCALf 2.99 9p450 10p537 10p539 12p576
NameCAL 2.92 5.200 5.207 8.391 8.394 8.399
NameCB4 2.91 5.198 5.206 8.389 8.398
name 2.75 5p197 5p202 5p220

noshow 1.20 5p190 9p486 10p559
nr 1.53 1.61 6.254 7.308 7.336 8.371 8.398 9.440
OldCanId 3.136 9p458 9.495 10=499 10=506
OpenEText 13.620
OpenFile 13.624
OutFile 1.41 5p192 5p194 10p510 10p516 10p521 10p527 10p534 10p535 10p536
10p541 13p624 14p675
obuf 1.42 13p625
ole 1.53 1.61 6.254 7.308 7.336 8.371 8.398 9.440
ParamCount 13.612 13.617 13.621
ParamStr 13.618 13.622
PrintEachCan 3.140 8.386 8.428 9.451 10.510 10.516 13=628 13=629
PrintMiss 3.140 8.393 9.435 13=636 13=637
PrintUnkn 3.140 8.395 9.437 13=632 13=633
ProcessACan <9.446 10.498 10.508
ProcessACluster <10.519 13.655
ProcessAFile <9.463 10.561
ProcessTotal <10.530 13.657
PtrText 1.40 9.470
par 1.53
pos 13.627 13.631 13.635 13.639 13.660 13.663 14.666
ReadEtxt 1.7
Red 13p607
Sig_Error <4.144 5.190 9.486 10.559
SPLTFileName 1.36 13=663
SpeciateConc <6.264 10.500 10.503 10.507
SplitFileRead 3.139 5=230 10.549 12=573
SplitLine 2.84
Splitline 2.73
SpltDefaultdir 1.34 12=571
SpNameString 2.68 2.91 2.92
StrIO 1.9
StrLib 1.8
showfile 1.19 4.144 4.153
single 2.78 2.79 9.466
sizeof 13.625
stop 1.18 5p190 9p486 10p559
switches 1.37 13p620 13p624 13p627 13p631 13p635 13p639 13p641
TextBackground 13.603
TextColor 13.605 13.607 13.609 13.613 13.645
TotCALf 2.97 9p450 10p537 10p539 12p576
TotCB4f 2.95 9p450 10p537 10p539 12p576
TotCNMHC 2.102 10p538 10p540
TotCount 2.101 9p450 10.532 10p537 10p540 12p577
TotLNMHC 2.102 10p538 10p540
TotNMHC 2.102 9p450 10p538 10p540 12p577
title 1.14 13p606
todays_date 1.31 5p192 12p584
todays_time 1.31 5p192 12p585
tol 1.53
UseLineCount 3.142 8.418 13=641 13=642
uCanCALf 2.128 7.313 7.337 9p454 9p457 9p460 12p582
uCanCB4f 2.126 7.310 7.336 9p454 9p457 9p460 12p582
uCfarray 1.61 2.96 2.106 2.116 2.126 6.242 7.324 7.344 8.405
uCluCALf 2.108 9p449 10p522 10p524 10p526 12p578
uCluCB4f 2.106 9p449 10p522 10p524 10p526 12p578
uFilCALf 2.118 9p448 10p511 10p513 10p515 12p580
uFilCB4f 2.116 9p448 10p511 10p513 10p515 12p580
uLfarray 1.62 2.98 2.108 2.118 2.128 6.244 7.326 7.346 8.407
un 1.53 1.58 2.91 5.206 5.208 6.252 6.296 7.334 7.357 8.368
8.389 9.431
uTotCALf 2.98 9p450 10p537 10p539 12p576

uTotCB4f	2.96	9p450	10p537	10p539	12p576				
version	1.16	13p610							
White	13p645								
Window	13.644								
writeln	13.606	13.608	13.610	13.611	13.652	14.671	14.679	14.682	14.683
xyl	1.53								
Yellow	13p605								
YY	3.137	8.412	8p427	9p458	9=476	10p514			
YYStr	3.137								
YYstr	2.71	8.412							
ZeroAcc	<6.241	9.460	10.515	10.526	12.576	12.578	12.580	12.582	